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NEWS
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10
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                 classification scheme
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                 Option to turn off MARPAT highlighting enhancements available
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                 has been enhanced and reloaded
                 CHEMLIST enhanced with new search and display field
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         NOV 20
                 additional databases
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         NOV 20
                 CA/CAplus to MARPAT accession number crossover limit increased
                 to 50,000
NEWS 23
         DEC 01
                 CAS REGISTRY updated with new ambiguity codes
         DEC 11
                 CAS REGISTRY chemical nomenclature enhanced
NEWS 24
                 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25
         DEC 14
         DEC 14
                 GBFULL and FRFULL enhanced with IPC 8 features and
NEWS 26
                 functionality
                 CA/CAplus pre-1967 chemical substance index entries enhanced
         DEC 18
NEWS 27
                 with preparation role
         DEC 18
NEWS 28
                 CA/CAplus patent kind codes updated
                 MARPAT to CA/CAplus accession number crossover limit increased
NEWS 29
         DEC 18
                 to 50,000
                 MEDLINE updated in preparation for 2007 reload
NEWS 30
         DEC 18
              NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
NEWS EXPRESS
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chain nodes :
7  9  18  19  22  23
ring nodes :
1  2  3  4  5  10  11  12  13  14  15
chain bonds :
1-22  1-23  2-7  4-18  4-19  5-9  9-10
ring bonds :
1-2  1-5  2-3  3-4  4-5  10-11  10-15  11-12  12-13  13-14  14-15
exact/norm bonds :
1-2  1-5  1-22  1-23  2-3  2-7  3-4  4-5  4-18  4-19  5-9
exact bonds :
9-10
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15
```

G1:H,CH3

G2:0,S

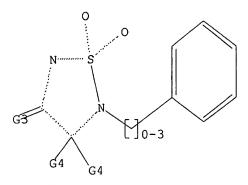
G3:0,S,N

G4:H,CH3

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0, S

G3 O, S, N

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 14:03:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 68 TO ITERATE

100.0% PROCESSED 68 ITERATIONS 50 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 866 TO 1854
PROJECTED ANSWERS: 576 TO 1424

L2 50 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 14:03:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1124 TO ITERATE

100.0% PROCESSED 1124 ITERATIONS 766 ANSWERS

SEARCH TIME: 00.00.01

I.3 766 SEA SSS FUL L1

=> fil hcaplus

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ENTRY SESSION

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=> s 13 L4 33 L3

=> d ed ibib abs hitstr 1-33

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 03 Aug 2006 ACCESSION NUMBER: 2006:765251 HCAPLUS DOCUMENT NUMBER: 145:211037

145:211037
Preparation of pyrazolyl aryl ureas as modulators of the protein kinase activation state for treatment of inflammation and hyperproliferative diseases Flynn, Daniel L.; Petillo, Peter A. Deciphera Pharmaceuticals, LLC, USA PCT Int. Appl., 30Spp.
CODEN: PIXXD2 TITLE:

INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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	PA'	TENT	NO.			KIN	D	DATE			APPL						ATE	
							-									-		
	WO	2006	0810	34		A2		2006	0803		WO 2	005-	US47	597		2	0051	223
		2006	0810	34		A3		2006										
		w:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	ΒY,	BZ,	CA,	CH,
			CN.	co.	CR.	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE.	GH.	GM.	HR.	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,
								LT,										
								NZ,										
			SG.	SK.	SL.	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
			VN,	YU,	ZA,	ZM,	ZW											
		RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF.	ÇG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
								NA,										
			vc.	K 7	MD	DIT	T.1	TM										

KG, KZ, MD, RU, TJ, TM PRIORITY APPLN. INFO.: US 2004-638987P P 20041223

OTHER SOURCE(S):

MARPAT 145:211037

Novel compds. and methods of using those compds. for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and

diseases
characterized by hypervascularization are provided. In a preferred

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

 $\begin{array}{lll} 872171-37-4 & HCAPLUS \\ Urea, N-[3-(1,1-dimethylethyl)-1-[3-[\{(3R)-3-methyl-1,1-dioxido-4-oxo-1,2,5-chiadiazoliddin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-maphthalenyl- (9CI) (CA INDEX NAME) \\ \end{array}$

Absolute stereochemistry.

872171-57-8 HCAPLUS

2-Naphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-0xo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl)- [9CI) | INDEX NAME

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) embodiment, the compds. of the invention modulate the activation state of p38 kinase protein, abl kinase protein, bcrabl kinase protein, braf kinase protein, bcrabl kinase protein. The compds. of the invention I have general formula (R1-(X))jm-A-NH-L-NH-D-(E)q-(Y)1-Q wherein R1 = aryl, heteroaryl, and heterocyclyl; and Y = individually O, S, alkynyl, alkenyl, etc.: A = an arom., monocycloheterocyclic; or bloycloheterocyclic ring; D = Ph or a 5-6-membered heterocyclic ring; E = Ph, pyridinyl, or pyrimidinyl; L = -(C)0- or -5(0)2-?; Jm, q,t = 0-1! and Q = a substituted ring or ring system. Over 500 compds. were prepd. For example, hydrogenation of 3-(3-aminophenyl) lacrylic acid Me ester provided the propionate, which was subsequently converted to the hydraxine. Reaction of the hydraxine with 4,4-dimethyl-3-oxopentamenitrile afforded Me
3-(3-text-butyl-5-amino-1H-pyrazole-1-yl)phenyllpropionate. which was coupled with 1-naphthyl isocyanate and reduced to provide urea II. In a competition assay with SKF 86002 as a fluorescent probe, II inhibited p38 MAP kinase with IC50

45 nM. 872171-35-2P, 1-[5-tert-Butyl-2-[3-[[(5)-3-methyl-1,1,4-trioxo-IT

[1, 2, 5] thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3- (naphthalen-1-yl]urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-{[(R]-3-nethyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3- (naphthalen-1-yl)urea 872171-57-8P, N-{3-tert-Butyl-1-[3-{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-{3-

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl}-3-(naphthalen-1-yl)urea 872171-63-6P, 1-{5-tert-Butyl-2-{3-

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl}-2H-pyrazol-3-yl}-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-methoxynaphthalen-1-yl)urea RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(p38 kinase inhibitor; preparation of pyrazolyl aryl ureas as

(938 kinase inhibitor; preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases)

RN 872171-35-2 MCRPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-({(35)-3-methyl-1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-62-5 HCAPLUS
Urea, N-{3-(1,1-dimethylathyl)-1-{3-({1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yi]methyl]phenyl}-1H-pyrazol-5-yl]-N'-1-maphthalenyl-(SCI) (CA INDEX NAME)

872171-63-6 HCAPLUS
Urea, N-(4-chlorophenyl)-N'-(3-(1,1-dimethylethyl)-1-[3-((1,1-dioxide-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-[4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

 $\begin{array}{lll} 872171-39-6 & HCAPLUS \\ Urea, & N-\{3-\{1,1-dimethylethyl\}-1-\{3-\{\{5-\{(4-methoxyphenyl\}methyl\}-1,1-(4-methoxyphenyl)\}methyl\}-1,1-(4-methoxyphenyl) \end{array}$

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl}-1H-pyrazol-5-yl}-N'-{4-fluorophenyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-[5-tert-Butyl-2-[3-[[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1],1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-[4],1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-[4-fluorophenyl)urea RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases)
RN 872171-36-3 HCAPLUS
CN Urea, N-[3-[1],-dimethylethyl)-1-[3-[[(3R)-5-[(4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSMER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 28 Jul 2006
ACCESSION NUMBER: 2006:739358 HCAPLUS
DOCUMENT NUMBER: 145:377543
TITLE: 15othiazolidinne heterocycles as inhibitors of protein tyrosine phosphatases: Synthesis and structure-activity relationships of a peptide

SCRUCLURE-ACTIVITY relationships of a peptide
Yue, Eddy W.; Wayland, Brian: Douty, Brent; Crawley,
Matchaw L.; McLauphlin, Erin: Takvorian, Amy;
Wasserman, Zelda: Bower, Michael J.; Wei, Min; Li,
Yanlong; Ala, Paul J.; Gonneville, Lucie: Wynn,
Richard; Burn, Timothy C.; Liu, Phillip C. C.; Comba,
Andrew P.
Discovery Chemistry, Experimental Station, Incyte
Corporation, Vilaington, DE, 19880, USA
Bioorganic & Hedicinal Chemistry (2006), 14(17),
5833-5849
CODEN: BMDCEP; ISSN: 0968-0896
Elsevier B.V.
Journal
English

CORPORATE SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: GI

Oxo- and trioxo-substituted isothiazolidinylphenylalanines are prepared

as
tyrosine mimetics by Suzuki coupling reactions of
chloroischiatolidinones
and chlorodioxoisochiatolidinones with N-Boc-4-borono-L-phenylalanine
derivs. the sochiatolidinylphenylalanines (with or without subsequent
hydrogenation) are incorporated into dipeptides prepared as human protein
tyrosine phosphatase 18 (PTPJB) inhibitors such as I. Of the compets,
tested, I is the most potent inhibitor of PTPJB with an IC50 value of 40
nM; the corresponding mixture of isothiatolidinone diastereomers inhibits
FTPJB with an IC50 value of 80 nM, and the separated
(R)-isothiatolidinone
diastereomer inhibits PTBJB with an IC50 value of 15.5 µM; the related

isothiazolidinone
diastereomer inhibits PTBLB with an IC50 value of 15.5 µM; the relat
dipeptides prepared inhibit PTPLB less potently than either I or the

mixture of isothiazolidine diastereomers containing I. Crystal structures of a

(Continued) ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

650315-21-8 HCAPLUS
L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl(5C1) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) dioxothiazolidinone-substituted dipeptide and a dioxoisothiazolinone-substituted dipeptide bound to PTPIB are detd. by X-ray crystallog.; the low energy conformation found by ab initio calens, for the satch the terocycle more closely approaches the conformation obtained upon

heterocycle more taboxy -pro-----binding
to PTPIB than that of the unsaid. heterocycle.

17 850315-22-99
R1: PAC (Pharmacological activity); SPN (synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(preparation of isothiazolone- and dioxoisothiazolone-substituted
phenylelanine-containing dipeptide amides and their activities as

n
PTP1B inhibitors)
850315-22-9 HcAPLUS
L-Phenylaleninamide, N-{{4-methoxyphenyl}acetyl}-L-phenylalanyl-4-(1,1dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-20-7P 850315-21-8P 850315-23-0P
910606-95-0P 910606-97-2P
Rt: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of isothiazolone- and dioxolothiazolone-substituted
phenylalanine-containing dipeptide amides and their activities as

PTP1B inhibitors)
850315-20-7 HCAPLUS
Carbamic acid, ([15]-1-[[4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thladiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

910606-95-0 HCAPLUS Benzenepropanamide, α -amino-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazoliddin-2-yl]-N-pentyl-, (αS) -, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 910606-94-9 CMF C23 H30 N4 O4 S

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

#1UbUb-97-2 HCAPLUS
L-Phenylalaninamide,
lenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]-N-pentyl-, mono(trifluoroacetate) [9CI] (CA
INDEX NAME)

CRN 910606-96-1 CMF C32 H39 N5 O5 S

Absolute stereochemistry.

CM 2

REFERENCE COUNT:

THERE ARE 39 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Title compds. (RlXj)mA(NH)pLn(NH)pDEqYtO [I; wherein Rl = (un)substituted (hetero)aryl: X, Y = independently O, S, NR6, NR6SO2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene,

O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h

1-4; $A = \{un\}$ substituted aryl, hetero(bi)cyclyl; $D = \{un\}$ substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; $E = \{un\}$ substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2;

m, n, p, q, t = independently 0, 1; Q = $\{un\}$ substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions]

prepared as p38 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p38 kinase protein comprises the step of contacting the α -C helix, the α -D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation

claimed, prepns. and/or characterization data for .apprx.150 examples of

and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl) acrylic acid Me ester using 10% Pd/C in EtOH provided

propionate, which was treated with NaNO2 in the presence of 6N HCl and SnC12~2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-[3-[3-tert-butyl-3-amino-1H-pyrazole-1-yl]phenyl]propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2C12, followed by reduction

LiOH in THF/MeOH/H2O provided the urea II. In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase

IC50 of 45 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data). 872171-35-2P, 1-[5-tert-Butyl-2-[3-{[(S)-3-methyl-1,1,4-trioxo-IT

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 672171-37-4P, 1-(5-tert-Butyl-2-[3-[(fR)-3-methyl-1,1,4-trioxo-{1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 672171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl)phenyl]-1H-pyrazol-5-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

[{1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1}methy1]pheny1]-2H-pyrazol-3-y1]-3-(naphthalen-1-y1)urea 872171-63-6P, 1-[5-tert-Buty1-2-[3-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 29 Dec 2005
ACCESSION NUMBER: 2005:1346235 HCAPLUS
DOCUMENT NUMBER: 144:88279
TITLE: Preparation of 1-pyrazolyl-3-phenylurea p38 MAP
kinase

inhibitors as antiinflammatory medicaments Flynn, Daniel L.; Petillo, Peter A. USA U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S. INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

	Ser. No. 746,460.						
DOCUMENT TYPE:	Patent						
LANGUAGE:	English						
FAMILY ACC. NUM. COUNT:							
PATENT INFORMATION:	·						
TAILMI INTOINENTION							
PATENT NO.	KIND DATE	APPLICATION NO.	DATE				

US 2005288286 US 2004180906 US 7144911	A1 20051229	US 2004-886329	20040706				
US 2004180906	A1 20040916	US 2003-746460	20031224				
US 7144911	B2 20061205						
WO 2006014290	A2 20060209	WO 2005-0523100	20050630				
WO 2006014290	A3 20060427						
W: AE, AG, AL,	AM, AT, AU, AZ, I	BA, BB, BG, BR, BW,	BY, BZ, CA, CH,				
CN, CO, CR,	CU, CZ, DE, DK, I	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,				
GE, GH, GM,	HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KM, KP, KR, KZ,				
LC, LK, LR,	LS, LT, LU, LV, 1	MA, MD, MG, MK, MN,	MW, MX, MZ, NA,				
NG, NI, NO,	NZ, OM, PG, PH, I	PL, PT, RO, RU, SC,	SD, SE, SG, SK,				
	TJ, TM, TN, TR,	TT, TZ, UA, UG, US,	UZ, VC, VN, YU,				
ZA, ZM, ZW							
RW: AT, BE, BG,	CH, CY, CZ, DE, I	DK, EE, ES, FI, FR,	GB, GR, HU, IE,				
IS, IT, LT,	LU, MC, NL, PL, I	PT, RO, SE, SI, SK,	TR, BF, BJ, CF,				
CG, CI, CM,	GA, GN, GQ, GW, I	ML, MR, NE, SN, TD,	TG, BW, GH, GM,				
KE, LS, MW,	MZ, NA, SD, SL, S	SZ, TZ, UG, ZM, ZW,	AM, AZ, BY, KG,				
KZ, MD, RU,	TJ, TM						
PRIORITY APPLN. INFO.:		US 2003-746460	A2 20031224				
		US 2002-437304P	P 20021231				
		US 2002-437403P	P 20021231				
		US 2002-437415P	P 20021231				
		US 2002-437487P	P 20021231				
		US 2003-463804P	D 20030418				
		US 2004-886329	A 20040706				
OTHER SOURCE(S):	MARPAT 144:88279						

OTHER SOURCE(S):

MARPAT 144:88279

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl|phenyl|-2H-pyrazol-3-yl}-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-{4-methoxynaphthalen-1-yl]urea Rl: PAC (Pharmacological activity); SPN (Synthetic preparation); THU [Therapeutic use]; BIOL (Biological study); PREP (Preparation); USES

(Therapoutic use): BIOL (Biological study): PREP (Preparation): USES (USes) (p38 kinase inhibitor; prepn. of (pyrazolyl)(phenyl)urea p38 kinase inhibitors as antiinflammatory agents) 872171-35-2 HCAPUS Urea, N-[3-1(1.7-dimethyl)entyl)-1-[3-[(35)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazoliddin-2-yl)methyl)phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-37-4 HCAPLUS Urea, N-[3-[1,1-dimethylethyl)-1-[3-[[(3R)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiaddszoliddin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry

872171-57-8 HCAPLUS

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
2-Naphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-[11,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-lH-pyrazol-5-yl]- (SCI) (CINDEX NAME)

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9CI) (CA INDEX NAME)

872171-63-6 HCAPLUS
Urea, N-(4-chlorophenyl)-N'-[3-[1,1-dimethylethyl]-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-[5-tert-Butyl-2-[3-[[5-(4-methoxybenzyl)-(R)-3-

Absolute stereochemistry.

872171-39-6 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-(3-[[5-({4-methoxyphenyl)methyl}-1,1-

1.4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y-]]methyl]phenyl]-1H-pyrazol-5-yl]-N'-[4-methoxy-1-nsphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-lH-pyrazol-5-yl]-N'-(4-fluorophenyl)- (9Cl) (CA INDEX NAME)

872171-49-8 HCAPLUS Urea, N-{3-(1,1-dimethylethyl)-1-{3-({1,1-dioxido-4-oxo-1,2,5-thiadiazoliddin-2-yl)methyl}phenyl}-1H-pyrazol-5-yl}-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

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L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Aug 2005
ACCESSION NUMBER: 2005:904352 HCAPLUS
DOCUMENY NUMBER: 143:248386
TITLE: Preparation of substituted arole derivatives for treating diseases mediated by PTPase activity
INVENTOR(S): Mjelli, Addan M. M.; Polisetti, Dharma R.;
Subramarian, Govindan; Quada, James C.; Atimilli, Murty N.; Yarragunta, Ravindra R.; Andrews, Robert Xie, Rongyuan
USA
U.S. Pat. Appl. Publ., 204 pp.
CODEN: USXXCO
Patent
English 1 PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. PATENT NO. KIND DATE APPLICATION NO. DATE

US 2005187277 A1 20050925 US:2005-56498 20050211
AU 2005214349 A1 20050901 AU 2005-214349 20050211
CA 2551909 A1 20050901 CA 2005-2551909 20050211
W: AE, AC, AL, AM, AT, AU, AZ, BA, BB, BB, CB, BR, BW, BY, BZ, CA, CM, CM, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GM, GM, HR, MI, UD, LI, LIN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MM, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PM, PL, PT, RO, RU, SC, SD, SE, SC, SK, SK, SY, TJ, TH, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VM, YU, ZA, ZM, ZM, RH; BW, GH, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZM, AZ, BY, KG, KZ, MD, RU, TJ, TH, AT, BE, BG, CH, CY, CZ, DE, DK, MR, NG, NG, GM, MG, MG, NG, GM, ML, MM, NG, NG, NG, GM, ML, MM, NG, NG, SD, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CH, GA, GM, GO, GM, ML, MM, NG, NG, NG, CM, MC, MG, NG, CG, CH, CH, CZ, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, LE, LS, LS, FI, FR, CB, GR, HU, LE, LS, LS, FI, FR, CB, CH, CY, CZ, DE, DK, EE, ES, FI, FR, CB, GR, HU, LE, LS, LI, LI, LT, LI, LI, LM, LM, NK, YU

PRIORITY APPLIN. INFO: US 2004-543971P P 20040212 DATE DATE KIND wo 2005-US4590 w 20050211

OTHER SOURCE(S):

MARPAT 143:248386

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

The title compds. I [a, b = 0-2; W = 0, S, NR2] (wherein R2 = alkyl,

); $R_1 = H$, halo, CN, etc.; L1 = a direct bond, (un)substituted NHCO, NHSO2, etc.; Ar1 = (un)substituted (hetero)aryl, fused cycloalkylaryl, etc.; Ar2 = (un)substituted (hetero)arylene, fused arylcycloalkylene, etc.; L2 = CHZ, O, alkylene, etc.; hxich can be useful as inhibitors of protein tyrosine phosphatases and thus can be useful for the management, treatment, control, or the adjunct treatment of diseases mediated by PTPase activity such as type I diabetes and type II diabetes, were

prepared Thus, treating

Thus, treating
4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl)-1Himidarole with Me bromoacetate followed by eater hydrolysis afforded 561
(4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl)-1H-imidarol-1yllacetic acid. The representative compds. I were tested for inhibition
of PTP-1B. In general, the exemplified compds. I may inhibit PTP-1B with
IC50 of less than 20 µM. The pharmaceutical compns. comprising the
compds. I, and their use in treating human or animal disorders are also
disclosed.
IT 863246-05-3P
863246-05-3P
RE. PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

863246-05-3P RI: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TMU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of substituted azole derivs. for treating diseases

(preparation of substitutes easily defined by PTPase activity)

RN 863243-91-8 MCAPLUS

CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4,4-dimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-57-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-{2,4-dichlorophenyl}]-2-[(1E]-2-[3'-(trifluoromethoxy)]1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

863245-74-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl)phenyl], 1,1-dioxide (9C1) (CA INDEX NAME)

Double bond geometry as shown.

863246-05-3 HCAPLUS Benzoic acid, $4-\{[4-(2,4-dichloropheny])-2-\{[1E]-2-[4-(1,1-dioxido-4-oxo-1,2,5-chiadia-zolidin-2-y])pheny]]etheny]-1H-imidazol-1-y]methy]-, methyl ester (9Cl) (CA INDEX NAME)$

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

C1

863243-80-5P 863243-92-9P 863243-91-0P
863243-94-1P 863243-95-2P 863243-96-0P
863244-06-8P 863244-07-9P 863244-08-0P
863244-13-7P 863244-47-7P 863244-18-13P
863244-52-4P 863244-53-5P 863245-52-4P
863245-56-1P 863245-58-3P 863245-52-4P
863245-56-1P 863245-61-8P 863245-52-9P
863245-61-0P 863245-61-8P 863245-62-9P
863245-61-0P 863245-61-8P 863245-63-P
863245-71-0P 863245-71-0P 863245-61-P
863245-11-0P 863245-71-0P 863245-61-P
863245-11-1P 863245-11-1P
863245-11-1P
863245-11-1P
863246-10-1P

(Uses)

(preparation of substituted azole derivs. for treating diseases mediated by PTPase activity)

RN 863243-80-5 HCAPLUS

CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-difluorophenyl)-2-[(1E)-2-(3'-(trifluoromethyl)[1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

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863243-94-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2-chlorophenyl])-2-[(1E)-2-(3'-trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-92-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-2,4,4-trimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863243-93-0 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 5-{4-{[4-pheny1-2-{(1E)-2-{3'-} (trifluoromethyl)|1,1'-biphenyl}-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-95-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{4-{[4-(4-chloropheny1)-2-{(1E}-2-{3'-trifluoromethyl)[1,1'-bipheny1]-4-yl]ethenyl}-1H-imidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-05-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 863244-06-8 HCAPLUS
(N 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(3,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-07-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(methylsulfonyl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazol-1-yl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-47-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[[3-(trifluoromethyl)phenyl]methyl]-1H-imidazol-1-yl]methyl!phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

N 863244-51-3 HCAPLUS N 1,2,5-Thiadiazolidin-3-one, 5-{4-{[4-{2,4-dichlorophenyl}-2-{2-{4-(trifluoromethyl)phenyl]=thyl]-1H-imidazol-1-yl]methyl]phenyl}-, L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Double bond geometry as shown.

RN 863244-08-0 HCAPLUS

(1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-[2-chloro-4-fluorophenyl]-2-[[1E]-2[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-13-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-{2,4-dichlorophenyl})-2-[[3'-

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-S2-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
C14-[[4-[2,4-dichiorophenyl]-2-[2-[2-fluoro-4(trifluoromethyl)phenyl]ethyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 863244-53-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[2-[3'-(trifluoromethoxy][1,1'-bipheny1]-4-yl]ethyl]-lH-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-25-4 HCAPLUS
CN Benzoic acid,
4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-56-1 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-{4-[(2-[(1E)-2-{3'-chloro[1,1'-biphenyl]-4-yl)ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl)methyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-60-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[[4-(2,4-dichlorophenyl)-2-[{1E}-2-[3'-(1-

methylethoxy) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], l,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

063245-61-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-{2,4-dichlorophenyl}}-2-[{1E})-2-[4'[(1-methylethyl)thio][[],1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-[(1E)-2-[3].5]bis(trifluoromethyl)fl,1'-biphenyl]-4-ylethenyl]-4-(2,4-dichlorophenyl)H-imidazol-1-yl}methyl)phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-58-3 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(IE)-2-(2'-fluoro-5'-propoxy[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-59-4 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl]methyl]phenyl]-, l,l-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-62-9 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 5-{4-[[4-(2,4-dichlorophenyl)-2-{(1E)-2-{4'-(1,1-dimethylethyl)[1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:continuous} \begin{array}{lll} 863245-63-0 & HCAPLUS \\ 1,2,5-thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dimehy]ethyl]-5'-methyl[[,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) \\ \end{array}$

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-64-1 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 5-{4-{[(2-{(1E)-2-{4-(5-chloro-2-thienyl)phenyl)-1-H-imidazol-1-yl]methyl)phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-66-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{2-[(1E]-2-[4-(5-acetyl-2-thienyl]phenyl]e-thenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-69-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(4,4,4-trifluorobutoxy)[1,1'-bipheny1]-4-y1]etheny1]-1H-imidazol-1-y1]methy1]pheny1}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-70-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-(2,4-dichlorophenyl)-2-[{1E}-2-[3'-

fluoro-4'-(4,4,4-trifluorobutoxy){1,1'-biphenyl}-4-yl|ethenyl}-1H-imiderol-1-yl|methyl|phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863245-67-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichlorophenyl)-2-{(1E)-2-[2'-fluoro-5'-(trifluoromethyl){1,1'-biphenyl}-4-yl]ethenyl}-1H-imidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-71-0 HCAPLUS
Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4oxo-1,2,5-thiadiazolidin-2-yl)phenyl|methyl]-1H-imidazol-2-yl]ethenyl]-4fluoro[1,1'-biphenyl]-3-yl]-, l-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-72-1 MCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichloropheny1)-2-{(1E)-2-{3'-(trifluoromethy)}|1,1'-bipheny1]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued) L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863245-75-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-{2,4-dichlorophenyl}-2-[(1E)-2-{2-

fluoro-4-(trifluoromethyl)phenyl)ethenyl]-1H-imidazol-1-yl]methyl)phenyl]-2-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-78-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{4-{4-(2,4-dichlorophenyl)-2-{(1E)-2-[4-(4,4,4-trifluorobucoxy)phenyl]ethenyl}-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(trifluoromethyl)phenoxy)phenyl|ethenyl|-1H-imidazol-1-yl}methyl|phenyl|-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-03-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{{4-(2,4-dichlorophenyl)-2-{(1E)-2-{3'-(methylsulfonyl){1,1'-biphenyl}-4-yl}ethenyl}-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-04-2 HCAPLUS

86J246-04-2 HCRPLUS
1,2,5-Thisdeiazolidin-3-one, 5-[4-[(1E)-2-[4-(2,4-dichlorophenyl)-1-ethyl1H-imidazol-2-yl]ethenyl]phenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Double bond geometry as shown.

RN 863245-80-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[4-[4-

(1,1-dimethylethyl)phenoxy]phenyl]ethenyl]-lH-imidazol-l-yl]methyl]phenyl]-, l,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-82-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-[4-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-06-4 HCAPLUS Benzoic acid, 4-[[4-{2,4-dichlorophenyl}]-2-[(1E)-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenyl]ethenyl]-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-07-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[4-{2,4-dichlorophenyl}-2-[{1E}-2-[3'-(methylsulfonyl)],1'-biphenyl]-4-yl]ethenyl]-lH-imidazol-1-yl]phenyl]-,1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-09-7 RCAPLUS Carbanic acid, $\{4'-[(1E)-2-[4-(2,4-dichloropheny1)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)pheny1]methy1)-1H-imidazol-2-y1etheny1][1,1'-bipheny1]-3-y1]-, 1-methy1ethy1 ester (9CI) (CA INDEX NAME)$

Double bond geometry as shown.

863246-10-0 HCAPLUS
Carbamic acid, [4'-[{1E}-2-{4-(2,4-dichlorophenyl}-1-[{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]methyl}-1h-imidazol-2yl]ethenyl][1,1'-biphenyl]-3-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Double bond geometry as shown.

863246-13-3 KCAPLUS
1,2,3-Thiadiarolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-phenoxyphenyl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide

(CA INDEX NAME)

Double bond geometry as shown.

 $\begin{array}{lll} 863246-15-5 & HCAPLUS \\ 1,2,5-Thiadiazolidin-3-one, & 5-\{4-\{\{4-\{2,4-dichlorophenyl\}-2-\{\{1E\}-2-\{3'-1\}\}\}\}\} \\ \end{array}$

(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-2-methylphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 863246-11-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1-

methylethyl) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-12-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-{2,4-dichlorophenyl}}-2-[(1E)-2-(3'-methyl[1,1'-biphenyl]-4-yl)ethenyl]-H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-16-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl)],1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-4-propyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863287-03-0 HCAPLUS
1,2,5-Thiadiarcolidin-3-one, 5-[4-[[4-(2,6-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 863247-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Reactant or reagent)
(preparation of substituted axole deriva. for treating diseases mediated by
PTPase activity)
RN 863247-41-0 RCRPLUS
ROBEROIC acid,
4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiaxolidin-2-yl)][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-, methyl ester (SCI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-89-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692764-94-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[1,1'-bipheny1]-3-yl-, 1,1-dioxide (9CI)
(CA INDEX NAME)

852835-44-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 May 2005
ACCESSION NUMBER: 2005:378875 HCAPLUS
DOCUMENT NUMBER: 143:19267
AUTHOR(5): Stucture-based design of protein tyrosine phosphatasp-1B inhibitors
Black, Emma: Breed, Jason; Breeze, Alexander L.; Embrey, Kevin; Garcia, Robert; Gero, Thomas W.; Godfrey, Linda; Kenny, Peter W.; Morley, Andrew D.; Minshull, Claire A.: Pannifer, Andrew D.; Read, Jon; Rees, Amanda; Russell, Daniel J.; Toader, Dorin; Tucker, Julie

CORPORATE SOURCE: AstraZeneca, Cheshire, SK10 4TG, UK
Bioorganic 4 Medicinal Chemistry Letters (2005), 15(10), 2503-2507
CODEM: BMCLES; ISSN: 0960-894X

DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 143:19267
AB Using structure-based design, a new class of inhibitors of protein tyrosine phosphataso-1B (PTP1B) has been identified, which incorporate the

1,2,5-thiadiazolidin-3-one-1,1-dioxide template.
692765-80-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-based design of protein tyrosine phosphatese-1B inhibitors)
692765-80-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

IT

612530-44-6P 692764-89-9P 692764-94-6P 852835-44-0P 852835-45-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (structure-based design of protein tyrosine phosphatase-1B inhibitors)

1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852835-45-1 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-(2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

142:4(1350
Preparation of 1-oxo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins Combs, Andrew P.; Yue, Eddy Wai Tsun; Bower, Michael Jason; Zhu, Wenyur Crawley, Matthew Lantz; Sparks, Richard Bruce; Pruitt, James Russell; Takvorian, Amy Incyte Corporation, USA
PCT Int. Appl., 329 pp.
CODEN: PIXXO2
Patent
English
1 INVENTOR(S)

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA*	TENT :	NO.			KIN										DATE					
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wo	2005	0355	51		A3		2006	0908												
	w -	AF.	AG.	AL.	AM.	AT.	AU.	AZ.	BA.	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,			
		CN.	co.	CR.	CU.	CZ.	DE.	DK.	DM.	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,			
		GE.	GH.	GM.	HR.	HU.	ID.	IL.	IN.	15.	JP,	KE,	KG,	KP,	KR,	KZ,	LC,			
		LK.	1.R	LS.	LT.	LU.	LV.	MA.	MD.	MG.	MK,	MN.	MW,	MX,	MZ,	NA,	NI,			
		NO.	NZ.	OM.	PG.	PH.	PL.	PT.	RO.	RU.	SC,	SD,	SE,	SG,	SK,	SL,	SY,			
		TJ.	TM.	TN.	TR.	TT.	TZ.	UA.	UG,	US,	υZ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
	BW:	RW.	GH.	GM.	KE.	LS.	MW.	MZ.	NA.	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,			
		AZ.	BY.	KG.	KZ.	MD.	RU.	TJ.	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,			
		EE.	ES.	FI.	FR.	GB.	GR,	HU,	IE,	IŤ,	LU,	MC,	NL,	PL,	PT,	RO,	SE,			
		SI.	SK.	TR.	BF.	BJ.	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,			
			TD.																	
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										U3 2	004	0003	001							

OTHER SOURCE(S): CASREACT 142:411350; MARPAT 142:411350

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention provides 1-oxo and 1,1-dioxoisothiazolones (shown

I-IV; also isothiazolidinone analogs of I-IV with R16 and R17 in place of R15 and Rz as a substituent at the 5 position of the isothiazolidinone ring: variables defined below. e.g. V) and related compds. that can modulate (no data) the activity of a target protein, such as a phosphatase, that selectively binds phosphorylated peptides or proteins. The present compds. can be useful (no data) in treating diseases or

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benrimidazol-2-yl]ethyl]biphenyl-4-sulfonamide 850315-36-5P 850315-00-1P, 4-Brono-N-[(1s)-2-(4-(1)-1d-ioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benrimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benrenesulfonamide trifluoroacetate 850315-48-5P, N-[(1s)-2-(4-(1)-1bioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benrimidazol-2-yl]ethyl]-3,5-bis[trifluoromethyl)benzenesulfonamide trifluoroacetate 850315-48-9P, N-[(1s)-2-(4-(1)-1bioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-biphenyl-4-sulfonamide trifluoroacetate 850315-65-0P 850315-69-4P

omo-N-[(1S)-2-[3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzensulfonamide trifluoroacetate 850315-73-0P, N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl)-3,5-bis[trifluoromethyl]benzensulfonamide trifluoroacetate 850327-65-0P 850327-67-2P, N-[(1S)-1-{5-chloro-1H-

benzimidazol-2-yl)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl}-2-cyanobenzenesulfonamide trifluoroacetate 850327-69-4P, N-{(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-71-8P,

N-{(15)-1-(5-Chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-73-0P, N-{(15)-1-(5-Chloro-1H-

benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenylethyl)-1,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-75-2P, N-{(18)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenylethyl)-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-77-4P, N-{(18)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenylethyl)-850327-79-6P, N-{(18)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenylethyl)-2-cyanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-{(18)-1-(1H-Benzimidazol-2-yl)-phenylethyl)-2-thiadiazolidin-2-yl)-phenylethyl-2-thiadiazolidin-2-yl)-phenylethyl-4-cyanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-{(18)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenylethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-83-2P, N-{(18)-1-(1H-Benzimidazol-2-yl)-

2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl)-3-phenoxybenzenesulfonamide trifluoroacetate 850327-85-47, N-{15}-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl)-3, 4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-69, N-{15}-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl)-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-89-89, 3-chloro-H-{15}-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-(3-chloro-1H-benzimidazol-2-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-2-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-1H-benzimidazol-3-yl)-3-(3-chloro-3-

benzimidazol-2-yl)-2-[3-chloro-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-fluorobenzenesulfonamide trifluoroacetate

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) disorders, including, for example, diabetes and obesity, that are connected directly or indirectly to the activity of the target protein. Methods of prepn. are claimed and hundreds of example prepns. are included. For example, V was prepd. in 12 steps (50, 62, 100, 59, not detd., 100, 100, 99, not detd., not detd., 43, and 25 % yield) starting from N-tert-butyl-3-[2-(tert-butylcarbamoyl)ethyldisulfanyl)propionamide. For I-IV: a dashed line indicates an optional bond; Sci is a lst mol. scaffold or is absent; Sc2 is a 2nd mol. scaffold or is absent, wherein

least one of Sc1 and Sc2 is present; or Sc1 and Sc2 together with X1 and X2 or X4 and X5 form a 5-, 6-, or 7-membered fused carbocyclic ring or a 5-, 6-, or 7-membered fused heterocarbocyclic ring; X1 is C or N when Sc1 is present; X1 is C or N to X2 is C or N when Sc2 is present; X2 is C or N when Sc2 is present; X2 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc1 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is present; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2, wherein the ring formed by X1, X2, X3, D1, D2, and D3 is an arom. ring; X4 is C or N when Sc1 is present; X4 is O, S, CR3, N, NR4,

CS, SO, or SO2 when Sc1 is absent; X5 is C or N when Sc2 is present; X5

O, S, CR3, N, NR4, CO, CS, SO, or SO2 when Sc2 is absent; X6 is C or N. Each El and E2 = O, S, CR3, N, NR4, CO, CS, SO, or SO2, wherein the ring formed by X4, X5, X6, El, and E2 is an arom. ring; R2 is H, halo, Cl-C4 alkyl, C3-C6 cycloalkyl, haloalkyl, OR3, SR28, NO2, CN, SOR29, SOZR29, COR3O, COOR31, NR3ZR33, a 5 - or 6-membered heterocarbocyclyl group, or tetrazolyl. R15 is H, halo, Cl-C4 alkyl, C3-C6 cycloalkyl, haloalkyl,

Cl-C4 alkoxy, Cl-C4 haloalkoxy, SH, Cl-C4-thioalkoxy, CN, NOZ, SO(Cl-C4 alkyl), SO(Cl-C4 haloalkoxy), SH, Cl-C4-thioalkoxy, CN, NOZ, SO(Cl-C4 alkyl), SO(Cl-C4 haloalkyl), SO2(Cl-C6 cycloalkyl), SONHZ, SO3H, SO2(Cl-C4 alkyl), SO2(Cl-C4 alkyl), SO(Cl-C4 alkyl), SO(Cl-C4 alkyl), CO(Cl-C4 alkyl), CO(Cl-C4 alkyl), CO(Cl-C4 haloalkyl), CONH(Cl-C4 alkyl), CONH(Cl-C4 alkyl), CONH(Cl-C4 alkyl), CONH(Cl-C4 alkyl), NOXH(Cl-C4 alkyl), NOXH(Cl-C4 alkyl), NOXH(Cl-C4 alkyl), NOXH(Cl-C4 alkyl), CONH(Cl-C4 alkyl), CONH(Cl-C4 alkyl), CONH(Cl-C4 alkyl), NOXH(Cl-C4 alkyl), NOXH(Cl-C4 alkyl), SO(Cl-C4 alkyl), SO(Cl-C4 alkyl), SO(Cl-C4 alkyl), SO(Cl-C4 haloalkyl), SO(Cl-C6 cycloalkyl), SONHZ, SO(Cl-C4 alkyl), SO(Cl-C4 alkyl), CO(Cl-C4 alkyl), CO(Cl-

C1-C4 haloalkyl), SO2(C3-C6 cycloalkyl), SO2NH2, CHO, COOH, CO(C1-C4 alkyl), CO(C3-C6 cycloalkyl), CO(C1-C4 haloalkyl), CO(heterocarbocyclyl), COO(C1-C4 alkyl), COO(C3-C6 cycloalkyl), COO(C1-C4 haloalkyl), CONHC1-C4 alkyl), CONHC1-C4 alkyl), CONHC1-C4 alkyl), CONHC1-C4 cycloalkyl), CON(C3-C6 cycloalkyl), NH(C1-C4 alkyl), NH(C3-C6 cycloalkyl), NH(C3-C

cycloalkyl), or N(C)-C6 cycloalkyl); or R16 and R17 together with the C atom to which they are attached form a C3-C6 cycloalkyl group or a 3-7 membered heterocycloalkyl group; and q1 is 1 or 2; addnl. details are given in the

Claims.

850315-19-4P. [(1S)-1-[(1S)-1-(Pentylcarbamoyl)-2-[4-[1,1,4-trioxo[1,2,5]thiadiarolidin-2-yl)phenyl]ethyl]carbamoyl)-2-phenylethyl]carbamoyl acid tert-butyl ester 850315-22-9P.

(2S)-2-[[2S]-2-([2-(4-Methoxyphenyl)acetyl]aminol-3-

phenylpropionyl}amino]-N-pentyl-3-[4-(1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]propionamide 850315-24-IP, N-[(1S)-2-[4-(1,1-Dioxido-4-

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
B50327-93-4P, N-[(1S)-1-(1H-Benzimidazo)-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)penyllethyl)-3chlorobenzenesulfonamide trifluoroacetate B50327-95-6P,
N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyllethyl)-3-fluorobenzenesulfonamide
trifluoroacetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(drug candidate: preparation) (drug candidate; prepn. of 1-oxo and 1,1-dioxoisothiazolone and

modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins such as phosphatases that bind phosphorylated \$850115-19-4 RCAPUUS L-Phenylalaninamide, N-{(1,1-dimethylethoxy)carbonyl}-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-22-9 RCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)-M-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

 $850315-24-1 \quad HCAPLUS \\ \{1,1'-Bipheny1]-4-sulfonamide, N-\{\{1S\}-2-\{4-\{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1\}pheny1\}-1-\{5-\{trifluoromethy1\}-1H-benzimidazol-2-y1\}ethy1\}- (9CI) \quad (CA INDEX NAME)$

(Continued) L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN Absolute stereochemistry.

RN 850315-36-5 HCAPLUS
CN Benzenesulfonamide,
N-((15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl]-4(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-35-4 CMF C25 H19 F6 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-43-4 CMF C26 H18 F9 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850315-48-9 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)phnyl]-1-[6-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2(trifluoromethoxy)-, mono(trifluoroacetate) [9CI] (CA INDEX NAME)

CM 1

CRN 850315-47-8 CMF C25 H19 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON SIN CMF C2 H F3 O2 (Continued)

850315-40-1 HCAPLUS
Benzenesulfonamide, 4-bromo-N-[(1S)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-39-8 CMF C25 H18 Br F6 N5 O6 S2

Absolute stereochemistry.

2

850315-44-5 HCAPLUS

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-63-8 HCAPLUS
[1,1'-Biphenyl]-4-sulfonamide, N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-

1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-62-7 CMF C30 H23 C1 F3 N5 O5 S2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

B50315-65-0 HCAPLUS
Bentenesulfonamide, N-[(13)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-4-(trifluoromethyl)-, mono(trifluoromethyl) (CA INDEX NAME)

CM 1

CRN 850315-64-9 CMF C25 H18 C1 F6 N5 O5 52

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-73-0 HCAPLUS
Benzenesulfonamide, N-[(|s]-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-72-9 CMF C26 H17 C1 F9 N5 O5 52

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850315-69-4 HCAPLUS
CN Benzeneaulfonamide,
4-bromo-N-[{15}-2-[3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]cthyl}-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-68-3 CMF C25 H17 Br C1 F6 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-65-0 HCAPLUS
CN Benzenesulfonamide,
N-{(!S)-1-{S-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-,
mono(trifluoroacetate) {9CI} (CA INDEX NAME)

CM 1

CRN 850327-64-9 CMF C23 H19 C12 N5 O5 52

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 850327-67-2 HCAPLUS

Senzenesulfonamide,
N-[[35]-1(-[3c-hloro-]H-benzimidazol-2-yl)-2-[3-chloro4-(1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl)phenyl]ethyl]-2-cyano-,
monofutifluoroacetate) [9C] (CA INDEX NAME]

CM 1

CRN 850327-66-1 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 02

850327-69-4 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-73-0 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-1-{5-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-3,4-dimethoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-72-9 CMF C25 H23 C12 N5 O7 S2

Absolute Stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide.
N-[(15)-1-{5-chloro-lH-benzimidazol-2-yl}-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME) CM 1 CRN 850327-68-3 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

2

RN 850327-71-8 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-{S-chloro-lH-benzimidazol-2-yl)-2-{3-chloro4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl}-3-phenoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-70-7 CMF C29 H23 C12 N5 O6 52

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-75-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-3,5-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-74-1 CMF C25 H23 C12 N5 O5 S2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-77-4 HCAPLUS

Benzenesulfonamide, N-{{|15}-1-{|14-benzimidazol-2-yl}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]ethyl]-,
mono(trifluoroacetate) (9Cl) (CA INDEX NAME)

CM 1

CRN 850327-76-3 CMF C23 H20 C1 N5 O5 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN (Continued)
Benzenesulfonamide, N=[(15]-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-80-9 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-83-2 HCAPLUS

Benzenesulfonamide, N-[{1S}-1-{1H-benzimidazo1-2-y1}-2-{3-chloro-4-{1,1-dioxido-4-oxc-1,2,5-thiadiazolidin-2-y1}pheny1}ethy1}-3-phenoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-82-1 CMF C29 H24 C1 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

F-C-CO2H

RN 850327-79-6 HCAPLUS

Renzenesulfonamide, N-{(15)-1-(1H-benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-2-cyano-,
mono(trifluoroacetate) (9C1) (CA INDEX NAME)

см 1

CRN 850327-78-5 CMF C24 H19 C1 N6 O5 52

Absolute stereochemistry.

2 CM

CRN 76-05-1 CMF C2 H F3 O2

CO2H

RN 850327-81-0 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2

CRN 76-05-1 CMF C2 H F3 O2

850327-85-4 HCAPLUS
Benzenesulfonanide, N-[{ls}-1-{lh-benzimidazol-2-yl}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenyl}ethyl}-3,4-dimethoxy-,mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-84-3 CMF C25 H24 C1 N5 O7 52

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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850327-87-6 HCAPLUS
Benzenesulfonamide, N-[{|1S}-1-{|1H-benzimidazol-2-yl}}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenyl}ethyl}-3,5-dimethyl-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-86-5 CMF C25 H24 C1 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

(Continued) ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

2 CM

CRN 76-05-1 CMF C2 H F3 O2

CO2H

850327-93-4 HCAPLUS Benzenesulfonamide, N-[(|15)-1-(|1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-chloro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-92-3 CMF C23 H19 C12 N5 O5 52

Absolute stereochemistry.

CH 2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850327-89-8 HCAPLUS
Benzenesulfonamide, 3-chloro-N-{(15)-1-(5-chloro-1H-benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl}-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-88-7 CMF C23 H18 C13 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

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Absolute stereochemistry.

RN 850327-91-2 HCAPLUS

Benzenesulfonamide,

N-[(15)-1-{5-chloro-1H-benzimidazol-2-yl})-2-{3-chloro-}

4-{1,-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl}phenyl|ethyl}-3-fluoro-,

mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-90-1 CMF C23 H18 C12 F N5 O5 S2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 76-05-1 CMF C2 H F3 O2

F-C-C02H

850327-95-6 HCAPLUS
Benzenezulfonamide, N-{(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4--oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]-3-fluoro-, monottrifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-94-5 CMF C23 H19 C1 F N5 O5 S2

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

r-c-co2H

IT 850315-20-7P, [(S)-2-[4-(5-Benzyl-1,1,4-

trioxo[1,2,5]thiadiazolidin-2-yl]phenyl]-1-(pentylcarbamoyl]ethyl]carbamic
 acid tert-butyl ester 850315-21-8P, {(1S)-1-{(1S)-2-(4-(5 Benryl-1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl]phenyl]-1 (pentylcarbamoyl)ethyl]carbamoyl)-2-phenylethyl]carbamic acid tert-butyl

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) ester 850315-23-0P, (25)-3-(4-(5-Benzyl-1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]-2-([(25)-2-[(2-(4-methoxyphenyl)acceyl)amino]-3-phenylpropionyl)amino]-N-pentylpropionamide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of 1-0xo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins) 850315-20-7 HCAPLUS Carbamic acid, ([(1S)-1-[(4-(1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)-2-oxo-2-(pentylamino)ethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-21-8 RCAPLUS L-Phenylalaninanide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl)-L-phenylalanyl-4-{1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM

ED Entered STM: 11 Apr 2005
ACCESSION NUMBER: 2005:308290 HCAPLUS
DOCUMENT NUMBER: 143:7658
AUTHOR(S): Expedient syntheses of sulfonylhydantoins and two six-membered analogs six-membered analogs and two six-membered analogs analogs

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

11

A range of α -amino esters can be turned into sulfonylhydantoins in a single, atom-economic step using sulfamide and DBU. E.g., reaction of BNHKCH2CO2Et with sulfamide and DBU gave 65% sulfonylhydantoin I. This procedure obviates the need for a three- or four-step sequence utilized

traditional procedures. Two new six-membered analogs (5-aryl-1,2,6-thiadiazinan-3-one 1,1-dioxides and 5-aryl-1,2-thiazinan-3-one 1,1-dioxides), e.g. II and III, have also been prepared utilizing novel synthetic protocols.
612528-23-1P 612529-46-1P 612530-69-5P 852358-50-0P 852358-51-3P 852358-55-3P 852358-54-4P 852358-56-9 852358-55-7-P
RL: SPN (Synthetic preparation); PREP (Preparation)

(Continued) L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (prepn. of sulfonylhydantoins via reaction of amino acid esters with sulfamide and DBU) 612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{2-phenylethyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

612529-46-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-bromophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

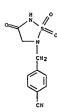
612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 852358-50-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-, 1,1-dioxide
(SC1) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-51-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2-methoxyphenyl)methyl]-, 1,1-dioxide (951) (CA INDEX NAME)

852358-53-3 RCAPLUS Benzonitrile, 4-{(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl}-(9C1) (CA INDEX NAME)



852358-54-4 HCAPLUS

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN



REFERENCE COUNT: THIS

THERE ARE 20 CITED REFERENCES AVAILABLE FOR 20

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
ethyl ester (9CI) (CA INDEX NAME)

852358-56-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{[1,1'-biphenyl]-3-ylmethyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

852358-57-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-methyl-5-(phenylmethyl)-, 1,1-dioxide, (45) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 08 Mar 2005 ACCESSION NUMBER: 2005:202894 HCAPLUS DOCUMENT NUMBER: 142:366767

142:365/67 1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides are potent inhibitors of human

AUTHOR (5):

heterocyclic sulfides are potent inhibitors of hum tryptase
Wong, Tzutshin; Groutas, Christopher S.; Mohan, Swathi; Lai, Zhong; Alliston, Kevin R.; Vu, Nga; Schechter, Norman M.; Groutas, William C. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Archives of Biochemistry and Biophysics (2005), 436(1), 1-7 CODEN: ABBIA4; ISSN: 0003-9861

CORPORATE SOURCE:

SOURCE:

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors describe herein the design, synthesis, and in vitro biochem.
Be the authors describe herein the design, synthesis, and in vitro biochem.
Cell-derived serine protesse tryptase. The inhibitors were readily obtained by attaching various heterocyclic thiols, as well as a basic primary specificity residue P1, to the 1,2,5-thiadiazolidin-3-one
1,1-dioxide scaffold. The inhibitors were found to be devoid of any inhibitory activity toward a neutral (elastase) or cysteine (papain) protease, however they were also fairly efficient inhibitors of bovine trypsin. The differential inhibition observed with trypsin suggests that enzyme selectivity can be optimized by exploiting differences in the S' subsites of the two enzymes. The results described herein demonstrate

versatility of the heterocyclic scaffold in fashioning mechanism-based inhibitors of neutral, basic, and acidic (chymo)trypsin-like serine

(1,2,5-Thiadiazolidin-3-one l,1-dioxide-based heterocyclic sulfides

are

potent inhibitors of human tryptase)
849415-30-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-2-[(2-benzoxazolylthio)methyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-31-2 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

849415-32-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-{((3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX INME)

Absolute stereochemistry.

849415-24-3P 849415-25-4P 849415-26-5P 849415-27-6P 849415-28-7P 849415-29-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

are

potent inhibitors of human tryptase)
849415-24-3 KCAPLUS
Carbamic acid, [4-{[35]-1,1-dioxido-4-oxo-2-{phenylmethyl}-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

849415-28-7 HCAPLUS
Carbamic acid, [4-[{35}-1,1-dioxido-4-oxo-2-{phenylmethyl}-5-[{{5-phenyl-1,3,4-oxadiazol-2-yl|thio|methyl}-1,2,5-thiadiazolidin-3-yl|butyl}-,
phenylmethyl ester [9CI] (CA INDEX NAME)

Absolute stereochemistry.

849415-29-8 HCAPLUS
Carbamic acid, {4-[(3S)-1,1-dioxido-4-oxo-2-{phenylmethyl}-5-[[(3-phenyl-1,2,4-oxadiazol-5-y)]thio]methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

849415-25-4 HCAPLUS
Carbamic acid, {4-{(35}-1,1-dioxido-4-oxo-2-(phenylmethyl)-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-3-yl]butyl}-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-26-5 HCAPLUS
Carbamic acid, [4-[(3S)-5-(chloromethyl)-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl|butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 849415-27-6 HCAPLUS
CN Carbamic acid,
{4+{(35)-5-{(2-benzoxazolylthio)methyl}-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl}butyl}-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 Aug 2004
ACCESSION NUMBER: 2004:677210 HCAPLUS
DOCUMENT NUMBER: 141:235669
Potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin-3-one 1,1 dioxide-based
sulfonamide derivatives
AUTHOR(S): Lai, Zhong; Gan, Xiangdong; Wei, Liuqing; Alliston,
Kevin R.; Yu, Hongyir Li, Yue H.; Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Archives of Biochemistry and Biophysics (2004),
429(2), 191-197
CODEN: ABBIA4; ISSN: 0003-9861
Elsevier
DOCUMENT TYPE: Journal

DOCUMENT TYPE: LANGUAGE:

English CASREACT 141:235669 OTHER SOURCE(S):

R SOURCE(S): CASREAUT 141:235669
The design, synthesis, and in vitro biochem. evaluation of a class of mechanism-based inhibitors of human leukocyte elastase (MLE) that incorporate in their structure a 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold with appropriate recognition and reactivity elements appended to it is described. The synthesized compds. were found to be efficient, time-dependent inhibitors of HLE. The interaction of the inhibitors with HLE is postulated to lead to the formation of a highly reactive ltonyl

time-dependent inhibitors of H.E. The interaction of the inhibitors with H.E. is postulated to lead to the formation of a highly reactive N-sulfonyl imine (a Michael acceptor) that arises from an enzyme-induced sulfonamide fragmentation cascade. Subsequent reaction ultimately leads to the formation of a relatively stable acyl enzyme. The results cited herein demonstrate convincingly the superiority of the 1.2.5-thiadiazolidin-3-one 1.1 dioxide scaffold over other scaffolds (e.g., saccharin) in the design of inhibitors of (chymoltrypsin-like serine proteases.

17 749866-31-07 749866-32-8P 749866-33-9P 749866-31-0P RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); TBU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (potent inhibition of human leukocyte elastase by 1,2,5-thiadiazolidin-3-one 1.1-dioxide-based sulfonamide derivs.)

RN 748866-31-7 RAPALUS
CN L-Phenylalanine, N-[[(145)-4-(2-methylpropyl]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 212331-99-2P 749866-30-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Proparation); RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
RN 212331-99-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

749866-30-6 HCAPLUS Ethanethioic acid, S-[{[45]-4-[2-methylpropyl]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester [9CI] (CA INDEX NAME)

Absolute stereochemistry.

IT 220869-64-7
RL: RCT (Reactant): RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by

1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)

RN 220869-64-7 RCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS OR STN (Continued)

749866-32-8 RCAPLUS
D-Phenylalanine, N-[[[(45)-4-[2-methylpropyl]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-33-9 HCAPLUS
L-Phenylalanine, N-{[[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}sulfonyl]-, phenylmethyl ester [9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-34-0 HCAPLUS
L-Phenylalanine, N-[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA
HDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

REFERENCE COUNT:

FORMAT

THERE ARE 36 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 30 Jul 2004
ACCESSION NUMBER: 2004:610081 HCAPLUS
DOCUMENT NUMBER: 141:157120
TITLE: Preparation of sulfahydantoins as phosphate isosteres for use as phosphateae inhibitors in the treatment of cancer and autoimmune disorders

INVENTOR(S): Saunders, Jeffrey O.; Miknis, Gregory F.; Blake,

INVENTOR(S): James

PATENT ASSIGNEE(S):

...
Vertex Pharmaceuticals Incorporated, USA
PCT Int. Appl., 62 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PA	TENT	NO.			KIND DATE				APPL		DATE								
	wo	2004	0626	64		Al		2004	0729		WO 2	003-	US 4 1	630		2	0031	230		
		W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	ÇA,	ÇH,	CN,		
			co.	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
			GM,	HR,	HU,	ID,	IL,	IN,	15,	JΡ,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,		
			LS.	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	OM,	PH,		
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	ΤZ,	ŲΑ,		
									ZM,											
		RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	ΤZ,	υG,	ZM,	ZW,	AM,	ΑZ,		
			BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	ВΣ,	BG,	CH,	CY,	cz,	DE,	DK,	EE,		
			ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,		
			TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,		
TG																				
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	ΑU	2003	3004	47		Al		2004	0810		AU 2	003-	3004	47		2	0031	230		
	ŲS	2004	1671	87		A1		2004	0826		US 2	003~	7491	21		2	0031	230		
	EP	1594	497			A1		2005	1116		EP 2	003-	8152	58		2	0031	230		
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			IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	ÇŹ,	EE,	Hυ,	sĸ			
	JP	2006	5149	60		T		2006	0518		JP 2	004-	5666	41		2	0031	230		
PRIC	RIT	YAPP	LN.	INFO	. :						US 2	002-	4375	72P		₽ 2	0021	230		
											WO 2	003-	US41	630		W 2	0031	230		

MARPAT 141:157120

OTHER SOURCE(5):

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
4-(1,1,4-Trioxo-[1,2,5]thiadiazolidin-2-yl)benzoic acid methyl ester
729600-47-9P 729600-48-0P 729600-49-1P
729600-50-4P 729600-51-5P 729600-52-6P
RL: PAC [PAramacological activity); SPN (Synthetic preparation); THU
(Therapoutic use); BIOL (Biological study); PREP (Preparation); USES (prepn. of sulfahydantoins as phosphate isosteres for use as protein

or phosphatase inhibitors in treatment of cancer and autoimmune

disorders)
RN 612527-99-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-,
methyl ester (9CI) (CA INDEX NAME)

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, S-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-44-6 HCAPLUS Benzoic acid, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl cater (9C1) (CA INDEX NAME)

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

The invention relates to compds. having a sulfahydantoin or a reverse sulfahydantoin moiety (I) and (II) or pharmaceutically acceptable salts thereof [Q = each (un)substituted Cl-8 aliphatic group, C6-10 argl, heteroargly having 5-10 ring atoms, heterocycly) having 3-10 ring atoms; T = Cl-6 alkylidene chain wherein one or two nonadjacent methylene units of T are optionally and independently replaced by O, NR, S, CO, CONR, NRCO, NRCONR, SO, SOZ, NRSOZ, SOZNR, or NRSOZNR; m = 0,1; X = CH2, CO, CF2: R = N or (un)substituted Cl-8 aliphatic group or two R groups bound to the

nitrogen are taken together with the nitrogen to form a 3-7 membered heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen,

heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen, ein said heteroatoms are independently selected from N, O, or S], uses thereof, and related methods. These compds, are inhibitors of phosphatases, particularly inhibitors of protein tyrosine phosphatase SHP-2 and are used in the treatment of various phosphatase mediated diseases such as proliferative diseases, autoimmune disorders, angiogenic disorders, and cancer. The autoimmune disease is selected from glomerulonephritis, rheumatoid arthritis, systemic lupus erythematosus, scleroderma, chronic thyroiditis, Graves' disease, autoimmune gastritis, diabetes, autoimmune hemolytic amenia, autoimmune neutropenna, thrombocytopenia, atopic dermatitis, chronic active hepatitis, mysathenia gravis, multiple sclerosis, inflammatory bowel disease, ulcerative colitis, Crohn's disease, psoriasis, or graft vs. host disease. The proliferative disease is selected from acute myelogenous leukemia, nic

proliferative disease is selected from acute myelogenous leukemia, chronic

myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple myeloma, and HTLV-1-mediated tumorigenesis. The angiogenic disorder is selected from solid tumors, ocular neovasculization, and infantile haemangionas. The cancer is selected from colon, breast, stomach, and ovarian cancer. Thus, N-alkylation of Me 4-aminobenzoate by Et bromoscetate in the presence of Et3N at 60° for 2.5 days gave 4-[([Ethoxycarbonyl)]methyl]maino]benzoic acid Me ester which underwent N-sulfamoylation by sulfamoyl chloride in the presence of Et3N in CH2Cl2 at room temperature overnight to give 4-[N-[(Ethoxycarbonyl)methyl]-N-sulfamoylamino]benzoic acid Me ester [III]. Cyclization of III by treatment with NaOMe/Meol at room temperature overnight gave 4-[1,1,4-trioxo-1,2,5-thiadiazolidin-2-yl)benzoic acid Me ester [IV]. IV showed ICSO of 1.0-100 µM against protein tyrosine phosphatase SRP-2.

IT 612527-99-8P 612530-69-5P 729600-44-6P,

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

729600-47-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME

729600-48-0 HCAPLUS
Benzoic acid, 3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, methyl ester (9C1) (CA INDEX NAME)

729600-49-1 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 5-(3-phenyl-2-propenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2-CH=CH-Ph

729600-50-4 HCAPLUS
Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

NH- (CH2)4-Ph

729600-51-5 HCAPLUS
Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

NH-CH2-Ph

729600-52-6 MCAPLUS Benzamide, N-butyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

DOCUMENT TYPE: LANGUAGE: FAMILY ACC, NUM. COUNT: English

PATE	NT :	NFOR	MATI	ON:														
	PA:	TENT :	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
							-									- 1		
	WO	2004	0603	05		A2		2004	0722		WO 2	003-	U541	425		2	0031	226
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		W:	AE.	AG.	AL.	AM.	AT.	AU,	ΑZ,	BA,	BB,	ВG,	BR,	BY,	BZ,	CA,	CH,	CN,
			co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JΡ,	ΚE,	KG,	ΚP,	ĸR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	OM,	PH,
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			UA,	UG.	US,	UŻ,	VC,	VN,	YU,	ZA,	ZM,	ZW						
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			BY.	KG.	KZ.	MD.	RU,	TJ,	TM,	AT,	ВE,	BG,	CH,	CY,	cz,	DΕ,	DK,	EE,
			ES.	FI.	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	5E,	SI,	SK,
			TR.	BF.	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,
TG																		
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	ΑU	2003 1590	3036	39		A1		2004	0729		AU 2	003-	3036	39		2	0031	226
	EP	1590	344			A2		2005	1102		EP 2	003-	8149	80		2	0031	226
		R:	AT.	BE.	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
									1017	CV	B T	TO	90	C 7	FF	1111	S.K.	
	BR	2003	0178	63		A		2005	1206		BR 2	003-	1786	3		2	0031	226
	CN	1756	849			А		2006	0405		CN 2	003-	8011	0049		2	0031	226
	CN	2003 1756 1791 2006 Y APP	596			A		2006	0621		CN 2	003-	8011	0048		2	0031	226
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PRIO	RIT'	APP	LN.	INFO	. :						US 2	002-	4373	0 4 P		P 2	0021	231
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											US 2	002-	4374	15P		P 2	0021	231
											U\$ 2	002-	4374	87P		P 2	0021	231

US 2003-463804P

US 2003-746545

US 2003-746607 WO 2003-US41425

P 20030418 A 20031224

A 20031224

W 20031226

MARPAT 141:140459 OTHER SOURCE(S):

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(Continued) ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Sulfamides, such as I, were prepared for use as anticancer agents which

by modulating the activation states of abl or bcr-abl α -kinase proteins. Thus, 4-MO2CC6H4CH2NNSCONKCOR [R = pyrrolidino], prepared from 4-Meo2CC6H4CH2NN2 and pyrrolidine, was treated with the pyrimidinylaminoaniline fragment to give I, which showed 10% inhibition

non-phosphorylated abl kinase at 10µM.
726192-44-5P 726192-45-6P 726192-60-5P
726192-61-6P
RL: PRC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
[preparation of sulfamides as anti-cancer agents)
726192-44-5 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-methyl]-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]- (9C1) (CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-ylmethyl]-N-[4methyl-3-{(4-phenyl-2-pyrimidinyl)amino|phenyl]- (9CI) (CA INDEX NAME)

726192-60-5 MCAPLUS
Benzamide, 4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yllmethyl]-N-[4-methyl-3-(2-pyrimidinylamino)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

726192-61-6 HCAPLUS
Urea, N-{4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]-N'-[4-methyl-3-(2-pyrimidinylamino)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612527-99-8P 612528-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfamides as anti-cancer agents)
612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-00-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 18 Jun 2004
ACCESSION NUMBER: 2004:93693 HCAPLUS
DOCUMENT NUMBER: 141:54348
Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as inhibitors of protein tyrosine phosphatase 1B

Kenny, Peter Wedderburn: Morley, Andrew David: Russell, Daniel John: Toader, Dorin
Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 48 pp.
COBEN: PIXXD2

DOCUMENT TYPE: Pater

DOCUMENT TYPE: LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT	NO.			KIN	0	DATE		- 2		ICAT:				D	ATE	
					-											
VO 2004	0506	46		Al		2004	0617	1	WO 2	003-0	GB51:	20		21	0031	126
W:	AE.	AG,	AL.	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	co.	CR.	CU.	ÇZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GE,
	GH.	GM.	HR,	KU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,
	LR.	LS.	LT.	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,
	OM.	PG.	PH.	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	sĸ,	SL,	SY,	TJ,	TM,
						UG,										
RW:						MW,									AM,	ΑZ,
	BY.	KG.	KZ.	MD,	RU,	TJ,	TM,	AT,	BE.	BG,	CH,	CY,	CZ,	DE,	DK,	EE,
	ES.	rı.	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	51,	SK,
						CI,										

AU 2003-302626 GB 2002-27813 20040623 AU 2003302626 PRIORITY APPLN. INFO.: Al

WO 2003-GB5120

OTHER SOURCE(S):

MARPAT 141:54348

Title compds. I [wherein Rl = H, (halogeno)alkyl, (hydroxy)alkoxy, alkylamino, etc.: R2 = H, (halogeno)alkyl, halogeno, alkoxy; R3 = alkylamido or (un)substituted alkyl; R4 = H, alkyl, (hetero)aryl; R5 = H

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN {Continued} Acetamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-3-methoxyphenyl]methyl]- {9CI} {CA INDEX NAME}

705256-61-7 HCAPLUS Butanamide, N-{{4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}pheny1}methy1}- {9CI} (CA INDEX NAME)

705256-67-3 HCAPLUS
Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-N-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) or alkyl; and pharmaceutically acceptable salts thereof] were prepd. as inhibitors of protein tyrosine phosphatase 1B (PTB1B). For example, 5-(4-(acctamidomethyl)-2-methoxyphenyl]-1,2. 5-thiadiazolidin-3-one 1,1-dioxide (II) was given in multi-step synthesis starting from 3-methoxy-4-nitrobenzyl alc. II showed inhibition of human PTB1B with ICSO value of 44pM. Thus, I and their pharmaceutical compns. are useful as inhibitors of protein tyrosine phosphatase 1B for the treatment of diabetes mellitus.

1T 705256-50-4P 705256-54-BP 705256-55-9P 705256-61-P7 705256-61-P 705256-61-P 705256-62-PP RDS256-19-P 705256-61-P 705256-62-PP RDS256-19-P RDS

(Uses)
(preparation of S-phenyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide derivs. as inhibitors of protein tyrosine phosphatase 1B)
RN 705256-50-4 HoAPLUS
CN Acetamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-54-8 HCAPLUS
Benzeneacetonitrile, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(5C1) (CA INDEX NAME)

705256-55-9 HCAPLUS

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 705256-72-0 HCAPLUS Benzenepentanamide, N-{[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-78-6 HCAPLUS Acetamide, N-[[4-(3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)phenyl]methyl)- (9CI) (CA INDEX NAME)

705256-82-2 HCAPLUS
Acetamide, N-[2-]4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

AcNH-CH2

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued) alkoxy, C1-6 alkoxy-C1-6 alkoxy, aryloxy, aryl-C1-6 alkoxy, aryloxy-C1-6 alkoxy, heteroaryl-C1-6 alkoxy, heteroaryl-C1-6 alkoxy, C1-6 alkoxy-C1-6 al

they are attached form a 5-7 membered carbocyclic or heterocyclic ring;

and R4 are selected such that (i) R3 = hydrogen, C1-6 alkyl, C1-6 alkyl, C1-6 alkylthio or halo and R4 = aryl, biaryl, heteroaryl, C2-6 alkynyl, C3-7 cyclosikyl, arylcarbonyl, heteroarylcarbonyl, aryl-C2-6 alkynyl, aryl-C2-6 alkynyl, c1-6 alkoxy, C1-6 alkyl, aryl-C2-6 alkynyl, aryl-C2-6 alkyl, aryl-C2-6 alkyl, aryl-C2-6 alkyl, bright (i) R4 = R, C1-6 alkyl, C2-6 alkynyl, C1-7 cyclosikyl, arylcarbonyl, heteroaryl, c2-6 alkynyl, C1-7 cyclosikyl, arylcarbonyl, heteroarylcarbonyl,

alkenyl, aryl-c2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6

aryl-C2-e
alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; Rb = H, C1-e
alkyl,
C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkyl, halo; R6 = H, C1-6 alkyl;
wherein any aryl, biaryl or heteroaryl group is optionally substituted]
are prepd. These compds are useful as inhibitors of protein tyrosine
phosphatase PTP1B for the treatment of diabetes mellitus. Thus,
4-tolylboronic acid was coupled with 5-(4-bromophenyl)-1,2,5thiadiazolidin-3-one in the presence of
tetrakis(triphenylphosphine)pallad
ium(0) [Pd(PPh3)4] and cesium carbonate in a mixt. of DMF, DME, EtOH, and
H2O at 170 for 600 s to give 5-(4'-Methyl-1,1'-biphenyl-4-yl)1,2,5-thiadiazolidin-3-one 1,1-dioxide.

IT 692765-08-5P 692765-17-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of phenylthiadiazolidinones as inhibitors of protein
tyrosine

phosphatase 1B (PTP1B) for treatment of diabetes mellitus) 692765-08-5 HCAPLUS (1,1'-Biphenyl)-4-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

692765-17-6 HCAPLUS [1,1'-Bipheny]-1-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9Cl) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 21 May 2004 ACCESSION NUMBER: 2004:412929 HCAPLUS DOCUMENT NUMBER: 140:423678
TITLE: Preparation of Fundamental Pr

phenyl)thiadiazolidin-3-

ones as inhibitors of protein tyrosine phosphatase 1B Birch, Alan Martin; Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 89 pp. CODEM: PIXXD2

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

PATENT :	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
					-											
WO 2004	0417	99		A1 20040521			1	WO 2	20031103							
W:	AE,	AG,	AL,	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN
						DK,										
						IL,										
	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ
	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	5G,	sκ,	SL,	5Y,	TJ,	TM
	TN,	TR,	TT.	TZ,	UA,	UĢ,	US,	UZ,	vc,	VN,	YU,	ZA,	ZM,	ZW		
RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ
						TJ,										
	ES.	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	sĸ
	TR.	BF.	BJ,	CF.	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD

GB 2002-25986 A 20021107 PRIORITY APPLN. INFO .:

w 20031103

OTHER SOURCE(S):

MARPAT 140:423678

AB The title compds. (I) or pharmaceutically acceptable salts thereof [Rl = H, halo, Cl-6 alkyl, Cl-6 alkoxy, Cl-6 alkylthio, halo-Cl-6 alkyl, halo-Cl-6 alkoxy, halo-Cl-6 alkylthio, hydroxy-Cl-6 alkoxy, dihydroxy-Cl-6

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-76-4P 692764-77-5P 692764-78-6P
692764-79-7P 692764-80-0P 692764-81-1P
692764-82-2P 692764-80-3P 692764-81-1P
692764-83-5P 692764-86-6P 692764-87-7P
692764-83-5P 692764-86-6P 692764-93-5P
692764-91-3P 692764-93-7P 692764-93-5P
692764-91-3P 692764-93-6P 692764-93-5P
692764-91-3P 692764-98-80-0P 692764-93-5P
692764-91-3P 692764-98-0P 692764-93-1P
692765-00-7P 692765-01-8P 692765-03-2P
692765-00-7P 692765-01-4P 692765-03-2P
692765-10-3P 692765-11-0P 692765-03-2P
692765-10-3P 692765-11-0P 692765-12-1P
692765-13-2P 692765-11-0P 692765-13-4P
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692765-13-2P 692765-13-6P 692765-13-4P
692765-30-1P 692765-13-6P 692765-13-4P
692765-30-1P 692765-30-3P 692765-31-4P
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692765-31-6P 692765-61-4P 692765-61-4P
692765-31-4P 692765-61-4P 692765-61-4P
692765-31-4P 692765-61-4P 692765-61-4P
692765-31-4P 692765-61-4P 692765-61-4P 692765-61-4P
692765-31-4P 692765-61-4P 69 (preparation of phenylthiadiazolidinones as inhibitors of protein tyrosine

phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
692764-76-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-77-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-nitro[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-78-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-dichloro[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-81-1 HCAPLUS
CN Acetamide, N-[4'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-3-yl]- (9CI) (CA INDEX NAME)

RN 692764-82-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-83-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (921) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-79-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-80-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2'-methyl{1,1'-biphenyl}-4-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN



RN 692764-84-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(methylthio){1,1'-biphenyl}-3-yl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692764-85-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (9c1) (CA INDEX NAME)

RN 692764-86-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-87-7 RCAPLUS Acetamide, N-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl){1,1'-biphenyl|-3-yl|-(3C1) (CA INDEX NAME)

692764-88-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[3-(2-benzofuranyl)phenyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

692764-89-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide [9CI] (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692764-93-5 HCAPLUS 1,2,5-Thiadiaolidin-3-one, 5-{1,1'-biphenyl}-4-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

692764-94-6 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

692764-95-7 HCAPLUS

esz.es=>5-7 RCAREUS 1,2,5-Thiadiazolidin-3-one, 5-[4'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-90-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-(5-oxazolyl)phenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

692764-91-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4-cyclohexylphenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

692764-92-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-benzoylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-96-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(4,4'-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-97-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-4'-phenoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-98-0 HCAPLUS CN [1,1"-Biphenyl]-3-carbonitrile, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-99-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-nitro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (gCI) (CA INDEX NAME)

RN 692765-00-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-01-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-hydroxy-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-05-2 HCAPLUS
CN Acetamide, N-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy(1,1'-biphenyl]-3-yl]- (9C1) (CA INDEX NAME)

RN 692765-06-3 HCAPLUS
CN 1,2,5-Thladiazolidin-3-one, 5-(4-methoxy-3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-07-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-02-9 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-(3',4,4'-trimethoxy{1,1'-bipheny1}-3-y1)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-4'-(trifluoromethyl){1,1'-biphenyl}-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-04-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[5-(1,3-benzodioxol-5-yl)-2-methoxyphenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 692765-09-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1E)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-10-9 HCAPLUS
CN 1,2,5-Thiadiazolididn-3-one, 5-[2-methoxy-5-[2-naphthalenyl)phenyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4'-(hydroxymethyl)-4-methoxy[1,1'-biphenyl)-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

N S CH2-OH

RN 692765-12-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

MeO.

RN 692765-13-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-14-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-4'-(phenylmethoxy){1,1'-biphenyl}-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

MeO CH2-OMe

RN 692765-19-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-20-1 HCAPLUS CN 1,2,5-Thiediazolidin-3-one, 5-(2'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (921) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO O-CH2-Ph

RN 692765-15-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(12]-2-phenylethenyl]phenyl]-, l,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Heo Z Ph

RN 692765-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-[(1,1-dimethylethoxy)methyl]-4-methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-,1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO N

RN 692765-22-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-difluoro-4-methoxy{1,1'-biphenyl}-3y1)-,1,1-dioxide (9CI) (CA INDEX NAME)

Meo Meo

RN 692765-23-4 HCAPLUS
CN 1,2,5-Thiadiazoliddin-3-one, 5-(5'-fluoro-2',4-dimethoxy{1,1'-biphenyl}-3-yl)-, 1,1-dioxide (9CT) (CA INDEX NAME)

N OM

RN 692765-24-5 HCAPLUS
CN 1,2,5-Thladdarolididn-3-one, 5-(4-methoxy[1,1':3',1''-terphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-25-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2'-fluoro-4-methoxy{1,1'-biphenyl}-3-yl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-27-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(1,1-dimethylethyl)-4-methoxy(1,1'-biphenyl)-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-32-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[(1E)-2-(4-chlorophenyl)ethenyl]-2methoxyphenyl]-1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-33-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-ethenyl-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-28-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy(1,1':4',1''-terphenyl)-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-29-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro-4'-fluoro-4-methoxy[1,1'-bipheny]1-3-y]1,-1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-30-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1':4',1''-terphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-furanyl)-2-methoxyphenyl]-,
1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-35-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-benzo[b]thien-2-yl-2-methoxyphenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{5-{2-benzofuranyl}-2-methoxyphenyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-37-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-acetyl-4-methoxy(1,1'-biphenyl)-3-yl)-,

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-38-1 HCAPLUS
CN (1.1'-Biphenyl)-3-carboxamide,
3'-(1.1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-39-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(1H-pyrazol-4-yl)phenyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-40-5 HCAPLUS
CN Pyrolidine, 1-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy([,1'-biphenyl]-4-yl]carbonyl)- (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-44-9 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, N-cyclohexyl-3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy-(9CI) (CA INDEX NAME)

RN 692765-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-amino-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 692765-46-1 HCAPLUS CN 1,2,5-Thiadiazolidin-1-one, 5-[4'-(dimethylamino)-4-methoxy[1,1'-biphenyl]-3-yl]-,1,1-dioxide (9C1) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-41-6 HCAPLUS CN (1,1'-siphenyl]-4-propanoic acid, 3'-(1,1-dioxido-4-oxo-1,2,5thiadiszolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-42-7 HCAPLUS
CN Carbamic acid, [[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl)-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 692765-43-8 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-47-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[4-pyridinyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-48-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-hydroxy-4-methoxy(1,1'-bipheny1}-3-y1)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-49-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-(1H-indol-6-yl)-2-methoxyphenyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-50-7 HCAPLUS
CN 1,2,5-Thiaddazolidin-3-one, 5-[2-methoxy-5-[2-thienyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-(phenylethynyl)phenyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-52-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(3-phenyl-1-propynyl)phenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-56-3 HCAPLUS

Enzoic acid, 2-[2-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

RN 692765-57-4 HCAPLUS
Benzoic acid, 2-[[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-4'-methoxy[1,1'-bipheny1]-3-y1]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-58-5 HCAPLUS
CN Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-yl]methoxy|-6-hydroxy- {9CI} (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-53-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{5-ethynyl-2-methoxyphenyl}-, 1,1-dioxide
(9C1) (CA INDEX NAME)

RN 692765-54-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methyl[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-55-2 HCAPLUS

Senzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipleny1)-3-y1]ethoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-59-6 HCAPLUS
CN Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-4-yl]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-60-9 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]ethoxy[-6-hydroxy- (9CI) (CA INDEX NAME)

RN 692765-61-0 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-62-1 HCAPLUS
Benzoic acid, 2-(3-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy(1,1'-biphenyl)-3-yl)propoxyl-6-hydroxy-(9C1) (CA INDEX NAME)

692765-63-2 MCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-64-3 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-4-yl]propoxy]-6-hydroxy-(9C1) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 692765-68-7 HCAPLUS
CN Benzoic acid,
2-[2-1[[3]"-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester (9C1) (CA INDEX NAME)

RN 692765-69-8 HCAPLUS
CN Benzoic acid,
2-[3-1[[3]"-[1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl)-4'methoxy[1,1'-blphenyl]-3-yl]carbonyl]amino]propoxy]-6-hydroxy-, methyl
ester (9C1) (CA IMDEX NAME)

RN 692765-70-1 HCAPLUS
CN Benzoic acid,
2-{[5-[[[]'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]pentyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-65-4 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1)propoxy}-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-66-5 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methoxy[-6-hydroxy- [9Cl) (CA INDEX NAME)

RN 692765-67-6 HCAPLUS CN [1,1'-Biphenyl]-3-carboxamide, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-mathoxy-N-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-71-2 HCAPLUS
CN Benzoic acid,
2-[[6-[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bjpheny1]-3-y1]carbony1]amino]hmxy1]oxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX NAME)

RN 692765-72-3 HCAPLUS
CN Benzoic acid,
2-{2-{[[[3'-{[1,-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-4'-methoxy[1,1'-biphenyl]-4-y1]carbonyl]amino]ethoxy}-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-73-4 MCAPLUS

Benzoic acid,
2-[3-{[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]carbony1]amino[propoxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-74-5 HCAPLUS
CN Benzoic acid,
2-[[5-[[3]"-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4"methoxy[1,1"-biphenyl]-4-yl]carbonyl]amino]pentyl]oxy]-6-hydroxy-, methyl
ester [9C1] (CA INDEX MAKE)

RN 692765-75-6 HCAPLUS
CN Benzoic acid,
2-{[6-{[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1}carbonyl]amino]hexy1]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

692765-79-0P 692765-80-3P 692765-84-7P
692765-85-8P 692765-86-9P 692766-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylthiadiazolidinones as inhibitors of protein

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN methoxyphenyl)- (9CI) (CA INDEX NAME) (Continued)

692765-86-9 HCAPLUS
1,2,5-Thladiazolidin-3-one, 5-[2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl]phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692766-02-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(5-iodo-2-methoxyphenyl)-, 1,1-dioxide (9CI)

(CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
RN 692765-79-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-80-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-84-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(5-bromo-2-methoxyphenyl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

692765-85-8 HCAPLUS Boronic acid, [3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 10 Oct 2003
ACCESSION NUMBER: 2003:796679 HCAPLUS

DOCUMENT NUMBER: 139:307766

TITLE: Preparation of substituted 1,1-dioxo-1,2,5-thiazolidine-3-ones as protein tyrosine phosphatase

and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis Coppola, Gary Mark, Davies, John William; Jewell, Charles Francis, Jr.; Li, Yu-Chin; Wareing, James Richard; Sperbeck, Donald Mark; Stams, Travis Mathew; Topiol, Sidney Wolf; Vlattas, Isidoros Novartis A.-G., Switz.; Novartis Pharma G.m.b.H. PCT Int. Appl., 148 pp. CODEN: PIXXD2 Patent English

INVENTOR(S):

ADDITION NO

DATE

PATENT ASSIGNEE(S): SOURCE:

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OTHER SOURCE(S): MARPAT 139:307766

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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Substituted thiazolidinetriones I [L1 = L2 = single bond, O1 = single bond, H, (un)substituted alkyl, cycloalkyl, or aminocarbonyl, carboxy, R1OC::O1, R1OCC:O1, R1OSC:O3, R1OCC:O3, R1OCC:O3, R1OCC:O3, R1OCC:O3, R1OCC:O4, R1OCC AB

: 7-membered ring interrupted by nitrogen, oxygen or sulfur atoms] such as II are prepared as inhibitors of protein tyrosine phosphatase 1b and

Il protein tyrosine phosphatase for overcoming insulin resistance and modulating glucose levels in the treatment or prevention of metabolic diseases, such as diabetes, or atherosclerosis. II is prepared by

treatment of Et bromoacetate with 1-naphthalenemethanamine, N-sulfamoylation with sulfamoyl chloride, and base-mediated cyclocondensation. No biol. data

is

provided.
612530-89-9P 612530-90-2P 612530-92-4P 612530-93-5P 612530-94-6P 612530-92-4P 612530-93-5P 612530-93-6P 612530-93-6P 612530-95-7P 612531-03-9P 612531-03-9P 612531-03-9P 612531-03-9P 612531-103-P 612531-03-9P 612531-13-2P 612531-13-3P 612531-13-4P 612531-23-4P 612531-23-4P 612531-33-69 612531-33-69 612531-33-69 612531-33-69 612531-33-69 612531-33-69 612531-61-67 612531-63-2P 612531-64-3P 612531-61-67 612531-66-5P IT

(Continued) 1.4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612530-92-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[(2,4-dimethoxypheny])=ethyl]-5-[(4-methoxy7-quinolinyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-93-5 HCAPLUS

CN Benzoic acid,
4-([5-([2, 4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, (4-(methylthio)phenyl)methyl ester (9CI)
(CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612531-67-6P 612531-68-7P 612531-69-8P
612531-70-1P 612531-71-2P 612531-72-3P
612531-73-4P 612531-75-6P 612531-76-7P
612531-77-8P 612531-78-9P 612531-79-0P
612531-60-3P 612531-69-4P 612531-79-0P
612531-60-3P 612531-69-4P 612531-79-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of thiazolidinetriones as protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or theosystems. And T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or theosystems.
612530-69-9 HCAPLUS
Carbmmic acid, [4-([5-([2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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RN 612530-90-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-{(2,4-dimethoxphenyl]methyl}-5-{(1-ethyl-2methyl-1H-benzimidazol-5-yl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-94-6 HCAPLUS
CN Benzoic acid,
-{{5-{(2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl)methyl}-, {4-{methylsulfonyl)phenyl|methyl ester (9CI) (CA INDEX NAME)

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612530-95-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{4-{bromomethyl}phenyl}methyl}-2-{{2,4-dimethoxyphenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-96-8 HCAPLUS Acetic acid, [[4-[[5-[(2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl[methyl]thio]-, ethyl ester [9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612530-98-0 HCAPLUS Acetic acid, [[4-[[5-[[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thicadiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(Continued)

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612530-99-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-iodophenyl)methyl]-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-00-7 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl)-, phonylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-01-8 HCAPLUS L-Phenylalanine, N-{{1,1-dimethylethoxy}carbonyl}-3-{{5-{{4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}(9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-05-2 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-10-9 HCAPLUS
CN Benzaldehyde,
4-[[5-[(2,4-dinethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiediszolidin-2-yl]methyl]- [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-02-9 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[(5-{(4-methoxyphenyl)methyl)-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-2-oxo-2(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-03-0 HCAPLUS Benzenepropanamide, α-amino-3-[[5-{{4-methoxyphenyl}methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}-N-pentyl-, (α5)-{9CI} (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-13-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-[[4-[(4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

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612531-22-3 HCAPLUS
Carbanic acid, [[4-[[5-{[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)

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612531-23-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612531-30-3 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-[[4-{aminomethyl}phenyl]methyl]-2-[(2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

RN 612531-24-5 HCAPLUS
CN Carbamic acid,
[2-{[4-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-th;adiazolidin-2-yl]methyl]phenyl]methyl]amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612531-31-4 HCAPLU5
CN Benzoic acid,
4-[[5-[[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

CH2 CH2 CH2

RN 612531-32-5 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, [4-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612531-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-(2,4-dinitrophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-35-8 HCAPLUS
N 1,2,5-Thiadiszolidin-3-one, 5-(2,4-diaminophenyl)-2-[(2,4-diaminophenyl)methyl)-, 1,1-dioxide (901) (CA INDEX NAME)

RN 612531-36-9 HCAPLUS
CN Benzoic acid, 3-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612531-61-0 HCAPLUS
CN 1H-1,4-Benzodiazepine-2,5-dione, 3-{[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-(phenylmethoxy)phenyl)methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 612531-63-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-64-3 HCAPLUS
CN L-Phenylalanine, N-[[1,1-dimethylethoxy]carbonyl]-4-[5-[[4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-65-4 HCAPLUS CN D-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-68-7 HCAPLUS
CN Benzenepropananide, α-amino-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadia2olidin-2-yl]-N-pentyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-69-8 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-[5-{(4-methoxyphenyl)methyl]-1,l-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-66-5 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-4-{5-{4-methoxyphenyl}methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-67-6 HCAPLUS
Carbamic acid,
[(1S)-1-[[4-[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl)-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-70-1 HCAPLUS
CN L-Phenylalanine, 4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 612531-72-3 HCAPLUS
CN L-Phenylalanine, N-acetyl-L-phenylalanyl-4-{5-[{4-methoxyphenyl}methyl}1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-73-4 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-[2-(1,1-dimethylethoxy)-2-oxoethyl]phenyl]ethyl]-4-[5-[(4-methoxyphenyl)methyl]-1,l-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-77-8 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-,phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-78-9 HCAPLUS
L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-3-[5-[4-methoxyphenyl]methyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-75-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-76-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(3-idophenyl)-2-((4-methoxyphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Con

RN 612531-79-0 HCAPLUS CN carbamic acid, [(15)-1-[(3-[5-(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiad[azolidin-2-yl]phonyl]methyl]-2-oxo-2-(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-80-3 HCAPLUS
CN Benzenepropanamide, α-amino-3-{5-{(4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-, (α5)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

612534-94-8 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

612527-93-2P 612530-46-8P 612530-49-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (invention compound; preparation of thiazolidinetriones as protein

sine
phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to
mitigate insulin resistance in the treatment of diabetes or
atherosclerosis)
612527-93-2 HCAPLUS
1,2,5-Thadiszolidin-3-one, 5-[(3-aminophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

ANSWER 14 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN 612527-98-7P 612528-00-4P 612528-01-5P 612528-02-6P 612528-07-1P 612528-01-5P 612528-02-6P 612528-07-1P 612528-01-6P 612528-10-6P 612528-11-7P 612528-12-8P 612528-13-9P 612528-23-1P 612528-13-9P 612528-23-PP 612528-23-PP 612528-23-PP 612528-23-PP 612528-23-PP 612528-23-PP 612528-23-PP 612528-23-PP 612528-33-PP 612528-33-PP 612528-33-PP 612528-33-PP 612528-34-PP 612528-33-PP 612528-33-PP 612528-34-PP 612528-33-PP 612528-34-PP 612528-33-PP 612528-35-PP 612528-6P 612528-6

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-46-8 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
ester (9CI) (CA INDEX NAME)

612530-49-1 HCAPLUS
Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-,
methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612530-04-8P 612530-05-9P 612530-06-0P
612530-08-2P 612530-09-3P 612530-10-6P
612530-11-7P 612530-12-8P 612530-13-9P
612530-16-2P 612530-12-3P 612530-13-9P
612530-22-0P 612530-23-3P 612530-25-3P
612530-22-0P 612530-23-3P 612530-25-3P
612530-22-9P 612530-33-3P 612530-21-1P
612530-32-2P 612530-33-3P 612530-31-1P
612530-35-9P 612530-33-3P 612530-31-4P
612530-31-3P 612530-31-3P 612530-31-4P
612530-31-3P 612530-31-3P 612530-31-4P
612530-31-3P 612530-31-3P 612530-31-5P
612530-44-6P 612530-42-4P 612530-43-5P
612530-44-6P 612530-65-4P 612530-47-9P
612530-49-0P 612530-50-4P 612530-51-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therspeutic use); BIOL (Biological study); PREP (Preparation); USES ses) (invention compd.; prepn. of thiazolidinetriones as protein tyrosine phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or

mitigate insulin resistance in the treatment of dispetes of atherosclerosis) 612527-84-1 KCRPUS 1,2,5-Thiadiazolidin-3-one, 5-(1-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-85-2 HCAPLUS Acetamide, N-(3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]pmethyl]- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612527-86-3 HCAPLUS
Carbamic acid, [[3-[[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]pheny1]methy1]-, 1,1-dimethy1ethy1 ester (9CI) (CA INDEX NAME)

612527-87-4 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-,: 1,1-dioxide (9C1) (GA INDEX NAME)

612527-88-5 HCAPLUS Acetamide, N-[{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1]pheny1]methy1}- (9CI) (CA INDEX NAME)

612527-90-9 HCAPLUS
Benzenepropanamide, N-[[4-[{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-ylmechyl]henyl|mechyl]- [9CI) (CA INDEX NAME)

612527-89-6 HCAPLUS
Carbamic acid, [[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612527-91-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(3-iodophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-92-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(3-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-94-3 HCAPLUS Acetamide, N-[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]mathyl]phenyl]- (9CI) (CA INDEX NAME)

(Continued) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612527-96-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(4-aminophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612527-97-6 HCAPLUS
Butanamide, N-{3-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}phenyl}- (9CI) (CA INDEX NAME)

RN 612527-98-7 HCAPLUS CN Urea, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-N'-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN propyl- (9CI) (CA INDEX NAME) (Continued)

612527-99-8 HCAPLUS
Benzoic acid, 4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9C1) (CA INDEX NAME)

612528-00-4 HCAPLUS Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-(9C1) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-07-1 HCAPLUS 1,2,5-ThiadisTolidin-3-one, 5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-08-2 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[(4-amino-2-bromophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-09-3 HCAPLUS
Acetamide, N-{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}phenyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-01-5 HCAPLUS
Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-(9CI) (CA INDEX NAME)

RN 612528-02-6 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-{(2-methylphenyl)methyl}-, 1,1-dioxide
(9CI)

(CA INDEX NAME)

(Continued) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-10-6 HCAPLUS
Methanesulfonamide, N-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]pheny1}- (9CI) (CA INDEX NAME)

612528-11-7 HCAPLUS
Methanesulfonamide, N-[[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]- {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)

RN 612528-12-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612520-13-9 HCAPLUS
CN Benzeneacetic acid, q-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-14-0 HCAPLUS
CN Benzeneacetamide, α-amino-2-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolldin-2-y1)methyl]-N-propyl- (9CI) (CA INDEX NAME)

RN 612520-15-1 HCAPLUS
CN Benzeneacetamide, α-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-16-2 HCAPLUS CN Benzeneacetamide, 4-[(1,1-d)xi(do-4-xo-1,2,5-thiadiazolidin-2-y1)methyl]-N-propyl- $\alpha-[(trifluoroacetyl)amino]- (9CI) (CA INDEX NAME)$

RN 612528-17-3 HCAPLUS
CN Benzeneacetamide,
4-[(1,1-dioxido-4-xo-1,2,5-thiadiazolidin-2-yl)methyl}α-[(methylsulfonyl)amino]-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-18-4 HCAPLUS
CN Benzenepropanamide, a-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)mothyl]-N-propyl- (9C1) (CA INDEX NAME)

RN 612528-19-5 HCAPLUS
CN Propanedioic acid, (acetylamino)[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

RN 612528-20-8 HCAPLUS
CN Benzenepropanamide, a-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thidalzolidin-2-yl]methyl]-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-21-9 HCAPLUS
CN Phenylalanine, N-acetyl-4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-26-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(2-chlorophenyl)ethyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-27-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(4-aminophenyl)ethyl]-, 1,1-dioxide
(9C1)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN (Continued)

RN 612528-22-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-α-phenyl-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-23-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-25-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3,4-dimethoxyphenyl)ethyl]-. 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

RN 612528-28-6 HCAPLUS CN Acetamide, N-{4-{2-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)ethyl]phenyl]-2,2,2-trifluoro-19C1) (CA INDEX NAME)

RN 612528-29-7 HCAPLUS
CN Butanamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-32-2 HCAPLUS CN 1,2,5-Thiadiazolidino-2-acetic acid, 4-oxo-α-(phenylmethyl)-, 1,1-dioxide (921) (CA INDEX NAME)

RN 612528-33-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 5-yl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-37-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxy-7-quinoliny1)methy1]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-38-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(2-methylpropoxy)-7-quinolinyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-39-9 MCAPLUS Glycine, N-[2-(butylamino)-2-oxo-1-phenylethyl]-N-[4-{(1,1-dioxido-4-oxo-1,2,3-thiadiazolidin-2-yl)methyl]benzeyl]- (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-34-4 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one, S-{{4-(aminomethyl)-1-naphthalenyl]methyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-35-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-((1-ethyl-2-methyl-1H-benzimidazol-5yl)methyll-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-36-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{[2-methyl-1-{3-methylbutyl}-1H-benzimidazol-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-40-2 HCAPLUS
CN Glycine, N-[2-(butylamino)-1-(4-ethylphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

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RN 612528-41-3 HCAPLUS
CN Glycine, N-[2-(butylamine)-2-exe-1-(3-phenoxyphenyl)ethyl]-N-[4-[(1,1-dioxide-4-exe-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612528-42-4 HCAPLUS
CN Glycine, N-[2-(butylamino)-1-(4-methoxyphenyl)-2-oxocthyl]-N-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Br

612528-44-6 HCAPLUS Glycine, N-[2-(butylamino)-1-(2-naphthalenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612528-45-7 HCAPLUS
CN Glycime, N-[2-(butylamino)-1-[4-chlorophenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

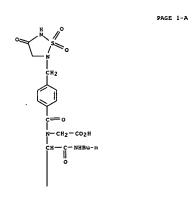
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RN 612528-43-5 HCAPLUS
CN Glycine, N-[1-(2-bromophenyl)-2-(butylamino)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)



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RN 612528-46-8 HCAPLUS
CN Glycine, N-[2-(butylamino)-2-oxo-1-[3-(phenylmethoxy)phenyl)ethyl]-N-[4[(1,1-dloxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA
INDEX NAME)

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O-CH2-Ph

RN 612528-47-9 HCAPLUS
CN Glycine,
N-[(2E)-1-[(butylamino)carbonyl]-3-phenyl-2-propenyl]-N-[4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 612528-48-0 HCAPLUS
CN Glycine,
N-[1-{(butylamino)carbonyl}-3-phenylpropyl}-N-[4-[(1,1-dioxido-4-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) PAGE 2-A

612528-50-4 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-, (3-chlorophenyl)methyl ester (9C1) (CA INDEX NAME)

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612528-51-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, (4-buxylphenyl)methyl əster (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-49-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(methylsulfonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612528-52-6 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, (4-(hydroymethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

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612528-53-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[2-(2-phenylethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [4-(difluoromethoxy)phenyl]methyl ester [9CI) (CA INDEX NAME)

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RN 612528-56-0 HCAPLUS
CN 2-Thiopheneacetic acid,
5-[{{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}}-n,a-difluoro-{9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-54-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[1,1'-biphenyl]-2-ylmethyl ester (9CI) (CA INDEX NAME)

612528-55-9 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-57-1 HCAPLUS Accetic acid, [{{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl|methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

612528-58-2 RCAPLUS Acetic acid. [[[4-[(1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-y]heethyl]phenyl]methyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)

RN 612528-59-3 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one,
5-[(4-[(3-methylbucyl)thio]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me2CH-CH2-CH2-S-CH2

RN 612528-60-6 HCAPLUS
CN Benroic acid, 4-(11,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-ethylbutyl seter (SCI) (CA INDEX NAME)

RM 612528-61-7 HCAPLUS CM Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-, cyclobucylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-64-0 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2,4,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

RN 612528-65-1 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-y1)methyl]-,
cyclohexylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-66-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl)methyl]-,
1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IN 612528-62-8 HCAPLUS
IN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, cyclopentylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-63-9 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl}methyl}-,
2-methylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-67-3 HCAPLUS
CN Benzoic acid, 4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
cyclopentyl ester (9CI) (CA INDEX NAME)

RN 612528-68-4 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2-methylbutyl ester (9C1) (CA IMDEX NAME)

RN 612528-69-5 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methylj-,
2-(methylthio)ethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-70-8 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-[(carboxymethyl)thio]ethyl ester (9CI) (CA INDEX NAME)

RN 612528-71-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-nitro-2-furanyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612528-74-2 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[3-(methylaulfonyl)phenyl)methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-72-0 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thlediazolldin-2-yl}methyl}-,
2-pyridinylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-73-1 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[3-(hydroxymethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612528-75-3 HCAPLUS
CN Benzeneacetic acid, 4-{4-{{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}benzoy1}amino|buty1}- (9CI) (CA INDEX NAME)

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612528-76-4 HCAPLUS
Benzeneacetic acid, 4-[3-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl|benzoy1]amino]propyl]- (9CI) (CA INDEX NAME)

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612528-77-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-[(dimethylamino)methyl]-2-furanyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-78-6 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612528-79-7 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(lH-indol-5-ylmethyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612528-80-0 HCAPLUS
1,2,5-Thiadicalidin-3-one, 5-[(3,4,5-trimethoxyphenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-82-2 HCAPLUS
1,2,5-Thiadizalidin-3-one, 5-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dloxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-83-3 HCAPLUS Benzeneacetic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyll- (SCI) (CA INDEX NAME)

612528-84-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-([4-benzoylphenyl]methyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-85-5 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-(2-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-86-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-[4-methyl-1-oxopentyl]phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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HO2C

RN 612528-89-9 HCAPLUS CN 2(1H)-Quinolinone, 6-[(1,1-dioxido-4-oxo-1,2,5-thiediazolidin-2-y1)methyl]-1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

612528-97-9 MCAPLUS
Acetamide, 2-amino-N-{[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]- (9CI) {CA INDEX NAME}

612528-98-0 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
{4-carboxyphenyl}methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-87-7 RCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[[3-(2-fluorophenoxy)phenyl]methyl]-,1-dioxide (9C1) (CA INDEX NAME)

612528-86-8 RCAPLUS
Benzoic acid, 3-{2-{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl|phenyl|ethoxy|- {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612528-99-1 HCAPLUS 1,2,5-Thiadiraclidin-3-one, 5-{(3-phenoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN [Continued] 612529-00-7 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methyl]-3-nitro- (9CI) (CA INDEX NAME)

612529-01-8 HCAPLUS . 1,2,5-Thiadiazolidin-3-one, 5-[[4-(hydroxymethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-02-9 HCAPLUS
Benzoic acid, 2-amino-4-((1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-05-2 HCAPLUS
Benzoic acid, 5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl)- (9CI) (CA INDEX NAME)

RN 612529-06-3 HCAPLUS CN 1,2,5-Thiadiszolidin-3-one, 5-[(4-chloro-3-methoxy-5-nitrophenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-03-0 HCAPLUS 1,2,5-Thiadiatolidin-3-one, 5-[(4-hydroxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-04-1 RCAPLUS Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-5-nitro- [9C] (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-07-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-08-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-methyl-2-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-09-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-, 1,1-dioxide

(CA INDEX NAME)

RN 612529-10-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-phenylpropyl)-, 1,1-dioxide (9CI) (CA

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) INDEX NAME)

RN 612529-11-0 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 5-[(4-butoxyphenyl)methyl)-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612529-12-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{{2-(trifluoromethyl)phenyl]methyl}-,
1,1-dioxide (9Cl) (CA INDEX NAME)

RN 612529-13-2 HCAPLUS CN Benzoic acid, 3-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)methyl- (921) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612529-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methyl-3-nitrophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX MAME)

RN 612529-17-6 HCAPLUS CN 1,2,5-Thiaddarolidin-3-one, 5-{(5-methyl-2-nitrophenyl)methyl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-aminophenyl)methyl]-, 1,1-dioxide (SCI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-14-3 HCAPLUS
CN Benzenebutanoic acid,
5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)- (9C1) (CA INDEX NAME)

RN 612529-15-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methyl-3-nitrophenyl)methyl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-19-0 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612529-20-1 RCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]phenyl]methyl)- (9CI) (CA INDEX NAME)

RN 612529-21-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[1,4-phenylenebis(methylene)]bls-, 1,1.1',1'-tetraoxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-22-3 HCAPLUS
CN Acetic acid, [[2-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)methyl]phenyl]amino]oxo- [9CI] (CA INDEX NAME)

RN 612529-23-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-hydroxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-24-5 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-28-9 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (921) (CA INDEX NAME)

RN 612529-29-0 HCAPLUS CN 1,2,5-Thladiazolidin-3-one, 5-[(3-amino-4-methylphenyl)methyl]-, 1,1-dioxide [9CI] (CA INDEX NAME)

RN 612529-30-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-amino-3-methylphenyl)methyl}-,
1,1-dioxide (8CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-fluoro-2-(trifluoromethy])phenyl]methyl}-, ll-dioxide (9CI) (CA INDEX NAME)

RN 612529-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612529-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-2-methylphenyl)methyl)-,
1,1-dioxide (921) (CA INDEX NAME)

RN 612529-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-([2-amino-5-methylphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-33-6 HCAPLUS CN Acetamide, N-[[4-(1].1-dioxido-4-oxo-1,2,5-thiadiatolidin-2yl]medhyl]phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

RN 612529-37-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-hydroxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612529-41-6 HCAPLUS CN Benzoic acid, 2-amino-5-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)methyl|-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-42-7 HCAPLUS

EN Benzoic acid,
2-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-43-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(phenylmethyl)phenyl]methyl]-,
1,1-dioxide [9C1] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-38-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3,5-dimethylphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-39-2 HCAPLUS
CN L-Phonylalanine, N-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]henyl]methyl]-, ethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-40-5 HCAPLUS
CN L-Phenylalanine, N-[[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-44-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-bis(trifluoromethyl)phenyl]methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4,6-trifluorophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-46-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-bromophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

(Continued) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-47-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5,5'-[[1,1'-biphenyl]-2,2'-diylbis[methylene]|bis-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

612529-48-3 HCAPLUS 1,2.5-Thiadiazolidin-3-one, 5-{{4-{(ethylamino)methyl}phenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-49-4 HCAPLUS

(Continued) ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Ph-CH2-CH2-NH-

612529-52-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-[(diethylamino)methyl]phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-53-0 HCAPLUS
Benzoic acid, 2-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid,
2-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl)- (9CI) (CA INDEX NAME)

612529-50-7 HCAPLUS
Benzoic acid, Z-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 612529-51-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[{4-[(2-phenylethyl)amino|methyl]phenyl]methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-54-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl]methyl}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 612529-56-3 MCAPLUS
CN Benzamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[2-[3{trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

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RN 612529-57-4 HCAPLUS CN Benzamide, 4-[[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methyl]-N-(3-methylbutyl)- (9C1) (CA INDEX NAME)

RN 612529-58-5 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-u-(phenylmethyl)-,
1,1-dioxide, (uS)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-59-6 HCAPLUS 1,2,5-Thiadiarolidine-2-acetic acid, 4-oxo- α -(phenylmethyl)-, 1,1-dioxide, (α R)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-63-2 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-64-3 HCAPLUS
CN Acetic acid, [4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenoxy}-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-60-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

RN 612529-61-0 HCAPLUS
CN Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 612529-62-1 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-65-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
{4-(carboxymethoxylphenyl)methyl ester (9CI) (CA INDEX NAME)

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612529-67-6 HCAPLUS
Benzoic acid, 4-[2-[[[4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]amino]ethyl]- (GA INDEX NAME)

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612529-73-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl)methyl)-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

612529-74-5 RCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-3-nitro-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue 612529-68-7 HCAPLUS Acetic acid, [4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenoxy]-, 2-methylpropyl ester (9CI) (CA INDEX NAME) (Continued)

612529-69-8 HCAPLUS Acetic acid, (4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y)]methyl]phenoxy]-, phenylmethyl ester (9CI) (CA INDEX NAME)

612529-70-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-75-6 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-3-nitro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

612529-76-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{4-ethoxyphenyl}methyl}-, 1,1-dioxide (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-77-8 HCAPLUS
CN 1,2,5-thiadiazolidin-3-one, 5-[[3-(trifluoromethyl)phenyl]methyl]-,
1,1-drioxide (901) (CA INDEX NAME)

RN 612529-78-9 HCAPLUS
CN Benzeneacctic acid, 4-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-80-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(phenylaminojethyl ester (9CI) (CA INDEX NAME)

RN 612529-81-4 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-y1)methyl)-,
2-(3-methoxyphenyl)ethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-79-0 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl]-,
2-phenylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-82-5 HCAPLUS

Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl)methyl
ester (9C1) (CA INDEX NAME)

RN 612529-83-6 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-84-7 RCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
3-methoxy-2,2-dimethyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

RN 612529-85-8 HCAPLUS

Senzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2,2,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-90-5 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl}-,
(3-methyl4--hittophenyl)methyl ester (9CI) (CA INDEX NAME)

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RN 612529-91-6 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-86-9 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}-,
3-{dimethylamino}-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-67-0 HCAPLUS

Enzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[(3aA,6,5,6,6a5)-5-(benzoyloxy)hexahydro-2-oxo-2H-cyclopenta[b]furan-4yl]methyl ester {9CI} (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (3-chloro-4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

c1

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RN 612529-93-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
6-ethoxy-6-oxohexyl ester (9CI) (CA INDEX NAME)

RN 612529-94-9 HCAPLUS
CN Benzoic acid, 4-{(l,l-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}2-(3-chlorophenyl)ethyl ester (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-(3-(trifluoromethyl)phenyl)ethyl ester (9CI) (CA INDEX NAME)

CF3

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RN 612529-97-2 HCAPLUS
CN D-Phenylalanine, N-[{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl}methyl}-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-98-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(phenylmethyl)amino]methyl)phenyl]meth L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-95-0 HCAPLUS CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-, 2-(3-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)

RN 612529-96-1 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) y1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-99-4 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

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612530-01-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)mothyl]-,
[4-(methoxycarbonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

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ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612530-03-7 HCAPLUS Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, 2-phenoxypropyl ester (9C1) (CA INDEX NAME)

612530-04-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(trifuoromethyl)phenyl]methyl ester [9C1) (CA INDEX NAME)

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612530-02-6 MCAPLUS
Benzoic acid, 4-[(l,l-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-cyclohexyl-2-methylpropyl ester (SCI) (CA INDEX NAME)

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612530-05-9 HCAPLUS Benzoic acid, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, [3-(trifluoromethyl]phenyl]methyl ester (9CI) (CA INDEX MAME)

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612530-06-0 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}-,
2-(4-carboxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612530-08-2 HCAPLUS
Benzoic acid, 3-[[[4-([1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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RN 612530-09-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(2-methylpropyl]amino]methyl]phenyl]me thyl]-,1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-10-6 HCAPLUS
CN 1.2.5-Thiadiaxolidin-3-one,
5-[{4-[(2.2-dimethylpropyl)amino|methyl]pheny
]|methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-11-7 HCAPLUS
Benzoic acid, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl]methyl]-,
1-naphthalenylmethyl ester [9CI] (CA INDEX NAME)

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612530-12-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
(4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612530-13-9 HCAPLUS
Benzeneacetic acid, 4-[2-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl)amino]ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612530-17-3 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyll-,
3-[(carboymethyl)minol-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-18-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

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612530-16-2 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
(3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-Thiophenecarboxylic acid, 5-{[[4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- [9CI) (CA INDEX NAME)

612530-19-5 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
{1,1'-biphenyl|-4-y1methyl ester (9CI) (CA INDEX NAME)

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RN 612530-20-8 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
[4-(acetylamino)phenyl|methyl ester (9CI) (CA INDEX NAME)

RN 612530-21-9 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
{2-(phenylmethyl)phenyl}methyl ester {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (2-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

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RN 612530-25-3 HCAPLUS

Senzeneacetic acid, 3-[[{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzyl]oxy]methyl]- (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-22-0 HCAPLUS
CN Benzoic acid, 4-[(I,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yi)methyl]-,
[2-methylphenyl]methyl ester (9C1) (CA INDEX NAME)

RN 612530-23-1 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,

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CH2-CO2H

RN 612530-26-4 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

N 612530-27-5 HCAPLUS

Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-fluoro-2-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

PAGE 1-A

RN 612530-28-6 HCAPLUS
CN Benzoic acid,
4-[5-[4,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl]phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2-0-C CH2-N S N-CH2-OM6

PAGE 1-B

_ OMe

RN 612530-29-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI)
(CA INDEX NAME)

N CH2 CO-CH2

RN 612530-30-0 HCAPLUS
CN Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
(5-methyl-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612530-31-1 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylphenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-33-3 HCAPLUS
Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
phenyl ester (9c1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612530-37-7 HCAPLUS
CN 1-Piperarineacetic acid, 4-(4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-ylmethyl]benzoyl]- (9C1) (CA INDEX NAME)

RN 612530-38-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
2-naphthalenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-34-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, [5-[(2-methyl)propyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-35-5 HCAPLUS
CN Benzole acid, 4-[(], 1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenylmethyl ester (9C1) (CA INDEX NAME)

RM 612530-36-6 HCAPLUS CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N,N-bis(2-methylpopyl)- (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-39-9 HCAPLUS
CN 2-Thiophenecarboxylic acid, 5-{[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]oxy]methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-40-2 HCAPLUS
CN Benroic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thizdiazolidin-2-yl)methyl)-,
[5-(aminocarbonyl)-2-thiznyl)methyl ester (9CI) (CA INDEX NAME)

RN 612530-41-3 HCAPLUS
CN Piperazine, 1-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-42-4 HCAPLUS
Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(1-oxo-3-phenylpropyl)-2-thianyl]methyl ester [9C1] (CA INDEX NAME)

612530-43-5 HCAPLUS

Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
[5-{((phenylmethyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA INDEX NAME

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-48-0 MCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{4-{aminomethyl}phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-50-4 HCAPLUS
CN Benzeneacetic acid, 2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)(9CI)

(CA INDEX NAME)

612530-51-5 HCAPLUS 1,2,5-Thladiazolidin-3-one, 5-(2,4-dimethoxyphenyl)-, 1,1-dioxide, potassium salt (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-45-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide (9CI) INDEX NAME)

612530-47-9 HCAPLUS Benzoic acid, 3-(1,1-dioxido-4-oxo+1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-52-6P 612530-53-7P 612530-54-8P 612530-55-9P 612530-55-P 612530-55-P 612530-57-1P 612530-65-P 612530-65-P 612530-65-P 612530-66-2P 612530-66-2P 612530-66-2P 612530-66-3P 612530-66-2P 612530-71-9P 612530-72-0P 612530-73-1P 612530-73-P 612530-7 612500-7 612530-7 612530-7 612530-7 612500-7 612500-7 612500-7 612500-7 61 RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation): USES {invention compound; preparation of thiszolidinetriones as protein tyrosine e phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or

atherosclerosis)
612530-52-6 HCAPLUS
Acetamide, 2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methylphenoxy}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

INDEX

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)

RN 612530-54-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-55-9 KCAPLUS CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-, phenylaethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-56-0 HCAPLUS CN L-Phenylalanine, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-60-6 HCAPLUS
CN L-Phenylalaninamids, N-benzoyl-0-(dicarboxymathyl)-L-tyrosyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-61-7 HCAPLUS
CN Benzenepropanamide, α-{{[1,1'-biphenyl}-4-ylsulfonyl)amino}-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl-, (αS)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued Absolute stereochemistry.

RN 612530-57-1 HCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl)-N-pentyl- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-58-2 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-59-3 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-(carboxymethyl)phenyl]ethyl]-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)- (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-62-8 HCAPLUS

CN Benzenepropanamide, a={((1,1'-biphenyl]-4-ylsulfonyl)amino]-4-{1,1-dioxidod-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)-, (aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-63-9 HCAPLUS

Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-a-[{phenylsulfonyl}amino}-, {aS}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-64-0 HCAPLUS
CN Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbuyl)-u-[(phenylsulfonyl)amino]-, (uS)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 612530-65-1 HCAPLUS
CN Benzenepropanamide,
4-(1,-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(3,3diphenylpropyl)-a-[(phenylsulfonyl)amino]-, (aS)- (9CI) (CA
INDEX MANE)

Absolute stereochemistry.

RN 612530-66-2 HCAPLUS
CN L-Phenylalaninamide,
N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo1,2,5-thladiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[(4-aminophenyl]methyl]-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612527-96-5 CMF C9 H11 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO2H

612530-72-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyl)-, 1,1-dioxide, mono(trifluoroacetate) (9C1) (CA INDEX NAME)

CRN 612528-35-5 CMF C13 H16 N4 O3 S

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-67-3 HCAPLUS Benzenepropanamide, 3-bromo-4- $\{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1\}-N-{4-phenylbutyl}-\alpha-{\{(phenylsulfonyl)amino}-, {\alphaS}-{9CI} {CA INDEX NAME} .$

Absolute stereochemistry.

RN 612530-68-4 HCAPLUS
CN L-Phenylalaninamide,
N-acetyl-L-phenylalaninyl-1-bromo-4-(1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-69-5 HCAPLUS 1,2,5-Thiadizolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-71-9 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-73-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[(2)-(3-oxo-2(3H)-benzofuranylidene)methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

612530-74-2 HCAPLUS Ethanedione, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]phenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-75-3 HCAPLUS 9,10-Anthracendione, 2-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl|methyl|- (9C1) (CA INDEX NAME)

612530-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide, sodium salt (9CI)

INDEX NAME)

612530-78-6 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide, trifluoroacetate (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 1

CRN 612530-45-7 CMF C8 H10 N4 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612534-93-7 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Ed Entered STN: 31 Jul 2002

ACCESSION NUMBER: 2002:55367 HCAPLUS
DOCUMENT NUMBER: 5137:232603

Efficient Solid-Phase Synthesis of Sulfahydantoins Tremblay, Melanie; Voyer, Normand; Boujabi, Sihem; Dewynter, Georges F.

Control de Recherche sur la Fonction, la Structure et l'Ingenierie des Proteines, Departement de Chimie, Faculte des Sciences et de Genie, Universite Laval, Quebec, OC, GlK 7P4, Can.

Journal of Combinatorial Chemistry (2002), 4(5), 429-435

CODEN: JCCHFF; ISSN: 1520-4766

American Chemical Society
JOURNET TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232603

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB A novel solid-phase strategy allows the efficient preparation of traceless sulfahydantoins. A total of 28 derivs., with crude purity generally higher than 85s, were prepared by parallel synthesis. Through reductive alkylations, Mitsunobu reactions, and sulfamoylation reactions on oxime resin, the synthetic strategy affords sulfahydantoin derivs. selectively substituted at N2, e.g., I, N5, e.g., II, and N2, N5, e.g., III, positions, although yields of disubstituted compds. are lower. The mild reaction conditions involved, lead to sulfahydantoins without racemization.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
459831-33-5P 459831-34-6P 459831-35-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of N2,N5-disubstituted sulfahydantoins

reductive alkylation of resin-bound phenylalanine with substituted benraldehydes and subsequent sulfamoylation, Mitsunobu reaction, resin-cleavage, and cyclization)
459831-33-5 KCAPLUS
1,2,5-Thiediazolidin-3-one,
459831-33-5 (APRUS)
459831-33-6 (APRUS)
459831-34-6 (

Absolute stereochemistry.

459831-34-6 HCAPLUS 1,2,5=Thladias-10idin-3-one, 2-butyl-5-((4-methylphenyl)methyl)-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 459831-35-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{{4-methylphenylmethyl}-4-{phenylmethyl}-2-{3-phenylpropyl}-, 1,1-dioxide, {45}- {9CI} {CA INDEX NAME}

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
283587-14-4P 459831-30-2P 459831-31-3P
459831-32-4P
REL SPN (Synthetic preparation); PREP (Preparation)
(secreoselective preparation of N5-substituted sulfahydantoins via (stereoselective preparation of N5-substituted suitangualitoris via
reductive
 alkylation of resin-bound phenylalanine with substituted benzaldehydes
 and subsequent sulfamoylation, resin-cleavage, and cyclization)
RN 283597-14-4 MCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methoxyphenyl)]methyl]-4-[phenylmethyl]-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME) Absolute stereochemistry.

459831-30-2 HCAPLUS
Benzonitrile, 4-{((3S)-1,1-dioxido-4-oxo-3-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

497031-31-3 MCAPLUS [1,2,5-Thidianalone, 5-[(4-nitrophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

n.ysp.r-y="q" mcArUus | 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Oct 2001 ACCESSION NUMBER: 2001:735235 HCAPLUS DOCUMENT NUMBER: 136:85785

A one-step protocol for the N-chloromethylation of heterocyclic imides Re, Shur Yu, Hongyir Fu, Qinghong: Kuang, Rongzer TITLE:

AUTHOR(S): Epp,

Epp.

Jeff B.; Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wachita State University, Wichita, KS, 67260, USA

SOURCE: Synthetic Communications (2001), 31(20), 3055-3058

CODEN: SYNCAV: ISSN: 0039-7911

PUBLISHER: Marcel Dekker, Inc.

JOURNAL JAMES BOUNCE(S): CASREACT 136:05785

AB A convenient single step methodol. for the N-chloromethylation of heterocyclic imides using a mixture of formaldehyde sodium bisulfite adduct

heterocyclic imides using a mixture of rormaturnyus social adduct and thionyl chloride is described. For example, the chloromethylation of 5-butyl-3-propyl-1, 2,5-thiadiazolidin-3-one 1,1-dioxide gave.

IT 387859-83-8 387859-86-1
RL: RCT (Reactant): RRCT (Reactant or reagent)
(preparation of 2-(chloromethyl)-1, 2,5-thiadiazolidin-3-one by chloromethylation of 1, 2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct)

RN 387859-83-8 (RAFMINS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 387859-86-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-,
phenylmethyl
ester, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9P 387859-88-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 30053-86-9 MCAPLUS

and formaldenyee sodium bluufite adduct;
300553-85-9 MCAPUUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

387859-88-3 HCAPLUS
1,2,5-Thiadiarolidine-3-acetic acid, 5-(chloromethyl)-4-oxo-2(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (901) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

(Continued) ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-07-8 HCAPLUS

CZYDOST-UT-D HANGUNG Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester [9CI) (CA

INDEX NAME)

RN 220869-14-7 KCAPLUS
CN Carbamic acid,
[2-{[{4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 220869-16-9 HCAPLUS
CN Carbanic acid,
[2-{[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 13 Jun 2001
ACCESSION NUMBER: 2001:426029 HCAPLUS
DOCUMENT NUMBER: 155:202665
ITITLE: Sulfonamides coupled to the
1.2.5-thiadiazolidin-3-one

1,2,5-thiadiazolidin-3

sulfonamides coupled to the one

1,1 dioxide scaffold
Groutas, W. C.; Ne, S.; Kuang, R.; Ruan, S.; Tu, J.;
Chan, H.-K.
Department of Chemistry, Wichita State University,
Wichita, KS, 67250, USA
Bioorganic & Hedicainal Chemistry (2001), 9(6),
1543-1548
CODEN: BMECEP; ISSN: 0968-0896
Elsevier Science Ltd.
Journal CORPORATE SOURCE:

CODEN: BMECEP: ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: Briglish

A A challenge associated with drug design is the development of selective inhibitors of proteases (serine or cysteine) that exhibit the same

primary
substrate specificity, i.e., show a preference for the same Pl residue.
While these proceases have similar active sites, nevertheless there are
subtle differences in their S and S' subsites which can be exploited. We
describe herein for the first time the use of functionalized sulfonamides
as a design and diversity element which, when coupled to the
1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold yields potent,
time-dependent inhibitors of the serine proteases human leukocyte

clastase
(HLE), proteinase 3 (PR 3) and cathepsin G (Cat G). Our preliminary findings suggest that (a) appending to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold recognition and diversity elements that interact with both the S and S' subsites of a target protease may result in optimal enzyme selectivity and potency and, (b) functionalized sulfonamades constitute a powerful design and diversity element with low intrinsic chemical reactivity and potentially wide applicability. Potent inhibitors of human leukocyte elastase, proteinase 3 and cathepsin G that interact with the S and S' subsites are realized by using functional sulfonamades coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold.

IT 220869-05-6P 220869-07-6P 220869-14-7P 220869-16-9P 365216-42-9P 365216-42-9P 365216-42-9P 365216-42-9P BESIL6-42-9P BESIL6-42-9P BESIL6-42-9P RESIL6-42-9P RES

ogical study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(Inhibition of serine proteases by functionalized sulfonamides coupled to 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)
220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl]-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA TNDEX NAME)

AMSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM (Continued) 1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]-2-oxoethyl)-, phenylmethyl ester (SCI) (CA INDEX NAME)

RN 365216-39-3 HCAPLUS
CN Benzamide,
N-[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5thiadiazolidin-2-yl]methyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

365216-41-7 HCAPLUS

RN 365216-41-7 HCAPLUS

Glycine

[[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carbonyl]-, ethyl ester

(9CI) (CA INDEX NAME)

365216-42-8 HCAPLUS

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN {Continued} Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis[phenylmethyl]-1,2,5-thiadiazolidin-2-yl]methyl}{phenylsulfonyl}-, butyl ester {9CI} {CA INDEX

365216-43-9 HCAPLUS L-Phenylalanine, N-{({{4S}-4-{2-methylpropyl}}-1,1-dioxido-3-oxo-5-

enylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carb onyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THIS

THERE ARE 35 CITED REFERENCES AVAILABLE FOR 35

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

(Continued) L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry

203587-15-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-16-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, -methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 RCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(4-(crifluoromethyl)phenyl]methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS

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L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Apr 2001
ACCESSION NUMBER: 2001:288468 HCAPLUS
DOCUMENT NUMBER: 135:76831
SYNTHASIS of a Sulfahydantoin Library
Albericio, Fernando: Bryman, Lois M.; Carcia, Javier;
Michelotti, Enrique L.; Nicolas, Ernesto; Tice, Colin
M.

CORPORATE SOURCE: Department of Organic Chemistry, University of
Barcelona, Barcelona, 08028, Spain
Journal of Combinatorial Chemistry (2001), 3(3),
230-300
CODEN: JCCHFF, ISSN: 1520-4766
PUBLISHER: American Chemical Society
Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 155:76831
AB A five-step solid-phase synthesis of sulfahydantoins from d-amino
acids and aldehydes was developed. The synthetic method allows the use
of
                                                                      A five-step solid-phase synthesis of sulfahydantoins from d-manno acids and aldehydes was developed. The synthetic method allows the use hindered amino acids, including Val, Phe, and Aib, and use of aromatic aldehydes substituted with electron-withdrawing and -donating groups. Some limitations were encountered with amino acids with reactive side chains. A small but diverse library of compds. was produced for biol. testing.

201507-14-0P 201507-15-5P 201507-16-6P 201507-18-BP 201507-18-P9 201507-18-P9 201507-19-P9 201507-21-PP 201507-2-P9 20
           and

aldehydes)

RN 283587-14-4 HCAPLUS

CN 1,2,5-Thiadiazolidin-3-one,

5-[(4-methoxyphenyl)methyl]-4-(phenylmethyl)-,

1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)
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L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (CO CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dihydro-1,4-henzodioxin-6-y1)methyl]-4- (1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiaddazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-ddoxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

283587-24-6 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[2(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-35-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(3-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-36-7 HCAPLUS Acctamide, N-[4-{[(3S)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-37-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-{l-methylethyl}-5-{(6-nitro-1,3-benzodioxol-5-yl)methyl}-,1,1-dioxide, {45}- {9CI} {CA INDEX NAME}

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) L4

346697-42-5 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[[4[phenylmethoxy]phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-43-6 HCAPLUS
Acetamide, N-[4-[[(3S)-1,1-dioxido-4-oxo-3-[{4-(phenylmethoxy)phenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346697-38-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-39-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[{2-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-40-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl}-4-{1-methylethyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-41-4 KCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[(4(phenylmethoxy)phenyl]methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

(Continued) ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

346697-45-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-[[4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-46-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{(2,4-dinethoxy-3-methylphenyl]methyl]-4-{[4[phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-47-0 MCAPLUS 1,2,3-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl)-4-{2-(methylthio)ethyl]-, 1,1-dioxide, (4SI- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

346697-49-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl)-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-49-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl)-4-[2-(methylthiolethyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-50-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl}4-[2-(methylthio)ethyl]-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
346697-55-0 HCAPLUS
1,2,5-Thiadiazolidin-1-one, 5-{(6-nitro-1,3-benzodioxol-5-yl}methyl)-4{(phenylmethyl)thiolmethyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-56-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4[[(phenylmethyllthio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-57-2 HCAPLUS
1,2,5-Thiadiatolidine-3-acetic acid, 2-[(3-chlorophenyl)methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (3CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-58-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 2-[[4-{acetylamino)phenyl]methyl}-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-51-6 MCAPLUS
1,2,5-Thiediarolidin-3-one, 5-((2-chlorophenyl)methyl)-4[((phenylmethyl)thio)methyl)-, 1,1-dioxide, (4R)- (5CI) (CA INDEX NAME)

$$Ph \longrightarrow S \longrightarrow R \longrightarrow O \longrightarrow C1$$

346697-53-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4[(5)benylmethyll+hio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-54-9 HCAPLUS Acetamide, N-(4-[[[3R]-1,1-dioxido-4-oxo-3-[[(phenylmethyl)thio|methyl]-1,2,5-lidaixorlidin-2-yllmethyl]phenyl]- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid,
2-{{4-chloro-3-nitrophenyl}methyl}-4oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-60-7 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[{2,4-dimethoxy-3-methylphenyl|methyl}-4-oxo-, phenylmethyl ester, 1,1-dioxide, {3S}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-62-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((4-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-63-0 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{1-methylethyl}-5-{{2-}
(trifluoromethyl)phenyl|methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. .

346697-64-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[{3-(trifluoromethyl)phenyl]methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-65-2 HCAPLUS
Benzoic acid, 4-[([35]-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-73-2 HCAPLUS
CN 1,2,5-Thiaddazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]4-[[4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (43)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-74-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{{3-methylphenyl}methyl}-4-{{1-(phenylmethyl)-1H-imidazol-4-yl}methyl}-, 1,1-dioxide, {45}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-([1-(phenylmethyl)-1H-imidazol-4-yl]methyl]-

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-69-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{3-methylphenyl)methyl}-4-[[4[phenylmethoxy)phenyl]methyl}-, 1,1-dioxide, (45)- {9CI} (CA INDEX NAME)

346697-71-0 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-[[4-(phenylmethoxy)phenyl]methyl]-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 346697-72-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-([2,3-dihydro-1,4-benzodioxin-6-yl]methyl]-4-[[4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-76-5 HCAPLUS
CN 1,2,5-Thiadiatolidin-3-one,
5-[(2,3-dihydro-1,4-ben:odioxin-6-y1)methy1]-4[[1-(phenylmethy1)-1H-imidaro1-4-y1]methy1]-, 1,1-dioxide, (45)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

346697-77-6 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-methylphenyl)methyl]-4-oxo-, methyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-79-8 HCAPLUS

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidine-3-acatic acid, 4-oxo-2-[{4(crifluoromethyl)phenyl]methyl]-, methyl ester, 1,1-dioxide, (35)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 346697-80-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-((2,3-dihydro-1,4-benzodioxin-6-yl)methyl)-4-oxo-, methyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

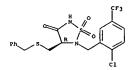
RN 346697-81-2 HCAPLUS
CN Acetamide, N-[4-[{(3S)-3-[2-(methylthio)ethyl]-1,1-dioxido-4-oxo-1,2,5- thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-82-3 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 4-(2-(methylthio)ethyl)-5-[(6-nitro-1,3-benrodioxol-5-yl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued



RN 346697-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- [9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(4-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-88-9 RCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-83-4 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-[(4-chlorophenyl)methyl)-4-[[(phenylmethyl)thio]methyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-84-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl)-4-[((phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-85-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl]phenyl]methyl]4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-89-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-{{2-chloro-5{trifluoromethyl]phenyl]nethyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide,
{35}- {9CI} (CA INDEX NAME}

Absolute stereochemistry.

RN 346697-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[(phenylmethoxy)methyl]-5-[[2-(crifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-91-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-{(phenylmethoxy)methyl}-5-{{3(crifluoromethyl)phenyl]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-92-5 HCAPLUS
Benzoic acid, 4-{[(33)-1,1-dioxido-4-oxo-3-[(phenylmethoxy)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-93-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl}-4-((phenylmethoxy)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-97-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{{4-nitrophenyl}methyl}-5-{{2-(trifluoromethyl)phenyl]methyl}-, 1,1-dioxide, (4\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346698-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-[[2-(trifluoromethyl)phenyl]methyl], 1,1-dioxide (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346698-04-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-phenyl-5-[(3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-05-3 HCAPLUS
Benzoic acid, 4-{[(33)-1,1-dioxido-4-oxo-3-phenyl-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

1.4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

346697-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[(3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-99-2 HCAPLUS
Benzoic acid, 4-{((35)-3-((4-nitrophenyl)methyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-00-8 HCAPLUS 1,2,5-Thiadiazolidin-2-one, 5-{(2,3-dichlorophenyl)methyl]-4-[(4-nitrophenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346698-06-4 HCAPLUS 1,2,5-Thiadiazolidin-1-one, 5-[{2,3-dichlorophenyl)methyl}-4-phenyl-1,1-dioxide, (43)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-12-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(4-methoxyphenyl)methyl}-4-{(15}-1-methylpropyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-14-4 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4-[(15)-1-methylpropyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 47 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 19 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Dec 2000
ACCESSION NUMBER: 2000:898004 HCAPLUS
DOCUMENT NUMBER: 134:307088
1,2,5-Thiadiazolidin-3-one 1,1 Dioxide: A Powerful Scaffold for Probing the S' Subsites of (Chymo)trypsin-Like Serine Protesses
AUTHOR(S): Ground, William C.; Epp, Jeffrey B.; Kuang, Rongze; Ruan, Sumei; Chong, Lee S.; Venkataraman, Radhike;

Tu,

Juan; He, Shu; Yu, Hongyi; Fu, Qinghong: Li, Yue He;
Truong, Tien M.; Vu, Nga T.

CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA

SOURCE: Archives of Biochemistry and Biophysics (2001),
385(1), 162-169

CODEN: ABBIA4; ISSN: 0003-9861

PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: Brglish
Brglish
English
English English English
English Engli

pages
in a predictable and substrate-like fashion. Consequently, inhibitors
derived from this heterocyclic scaffold interact with both the S and S'
subsites of an enzyme. Exploitation of binding interactions with both

S and S' subsites of a target enzyme may lead to compds. With greatly enhanced enzyme selectivity and inhibitory potency. This preliminary report describes the use of a series of compds having the heterocyclic scaffold linked to various amino acids to probe the S' subsites of human leukocyte elastase (HLE), proteinase 3 [PR 3], and cathepsin G (Cat G). For comparative purposes, a series of compds. derived from a related scaffold, isothiazolidin-3-one 1,1 dioxide (II), was also generated. Several of the compds. were found to be highly potent and selective time-dependent inhibitors of HLE, PR 3, and Cat G. (c) 2001 Academic Press.

Tress. 334975-68-7P 334975-69-8P 334975-75-6P 334975-61-4P 334975-83-6P 334975-85-8P 334975-88-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical
study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold for probing S'
subsites of human leukocyte elastase, proteinase 3 and cathepsin G)
334975-68-7 HCAPLUS
L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

334975-81-4 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl)-, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

334975-83-6 HCAPLUS
L-Phenylalanine, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester, monohydrochloride (5C1) (CA INDEX

NAME)

Absolute stereochemistry.

● HCl 334975-85-8 HCAPLUS L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

334915-69-8 HCAPLUS
D-Phenylalanine, N-{{1,1-dimethylethoxy|carbonyl}-, {445}-4-{2-methylproyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

334975-75-6 HCAPLUS L-Phenylalanine, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 334975-74-5 CMF C23 H29 N3 O5 5

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(4S)-1,1-dioxido-3oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazclidin-2-yl)methyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

334975-88-1 MCAPLUS
D-Phenylalanine, [(45)-1,1-dioxido-3-oxe-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 334975-87-0 CMF C26 H27 N3 O5 S

Absolute stereochemistry.

2

CRN 76-05-1 CMF C2 H F3 O2

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR

REFERENCE COUNT:

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl-2-oxazolyl)thio]methyl]-4-[2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-[{(5-phenyl-1,3,4-oxadiazol-2-yl]thio|methyl]-, 1,1-dioxide (9CI) (CA INDEX

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Jul 2000
ACCESSION NUMBER: 2000:488727 HCAPLUS
DOCUMENT NUMBER: 133:277919
Potent inhibition of serine proteases by heterocyclic sulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1 digital d aulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1
dioxide
AUTHOR(S): He, S.; Kuang, R.; Venkataraman, R.; Tu, J.; Truong,
T. M.; Chan, B. K.; Groutas, W. C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bisorganic Medicinal Chemistry (2000), 8(7),
1113-1217

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Blaswier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 133:277919

AB The existence of subtle differences in the Sn' subsites of
Clossly-related
(Chymoltrypain-like serine proteases, and the fact that the
1,2,5-th:addiazolidin-3-one 1,1 dioxide scaffold docks to the active site
of (chymoltrypain-like enzymes in a substate-like fashion, suggested
that the introduction of recognition elements that can potentially interact with the Sn' subsites of those proteases might provide an effective means for optimizing enzyme potency and selectivity. Accordingly, a series of heterocyclic sulfide derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) was synthesized and the inhibitory activity and selectivity of these compds. toward human leukocyte elastase (HLE), proteinase 3 (PR 3) and cathepsin G (Cat G) were then determined dis. With Pl=isobutyl were found to be potent, time-dependent inhibitors of HLE to a lesser extent PR 3, while those with Pl=benzyl inactivated Cat G rapidly and irreversibly. This study has demonstrated that 1,2,5-thiadiazolidin-3-one 1,1 dioxide-based heterocyclic sulfides are effective inhibitors of (chymolrtypsin-like serine proteases. 220869-26-1P 220869-27-2P 220869-29-4P 220869-33-DP 220869-33-DP 220869-33-PP 220869-38-SP 220869-38-SP 220869-38-SP 220869-38-SP 220869-39-GP 220869-40-SP RL: BAC (Biological activity or effector, except adverse); BSU logical and, logical
study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)
(potent inhibition of serine proteases by heterocyclic sulfide derivs.
of thiadiazolidinone dioxide) (Biological

220869-26-1 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(2-benzoxazolylthio)methyl}-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 220869-30-7 HCAPLUS 1,2,5-Thiaddazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio|methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-J5-2 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-2-([(5-phenyl-2-benzoxazolyl)thio]methyl]-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-39-6 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-(((5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-40-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{(6-amino-2-benzoxazolyl)thio]methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9 RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of thiadjazolidinone dioxide derivative; potent inhibition

serine proteases by heterocyclic sulfide derivs. of thiadiazolidinone dioxide)

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 15 Jun 2000
ACCESSION NUMBER: 2000:395930 HCAPLUS
DOCUMENT NUMBER: 133:159638
TITLE: Utilization of the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold in the design of potent inhibitors

οf

AUTHOR(S):

serine proteases: SAR studies using carboxylates Kuang, R.; Epp. J. B.; Ruan, S.; Chong, L. S.; Venkataraman, R.; Tu, J.; He, S.; Truong, T. M.; Groutas, W. C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (2000), 8(5), 1005-1016
CODEN: BMECEP; ISSN: 0968-0896
Elsevier Science Ltd.
Journal CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

ISBER: Elsevier Science Etc.

MENT TYPE: Journal

UAGE: English
A series of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one
1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds has been
synthesized and the inhibitory profile of these compds. toward human
leukocyte elastase (HEE), cathepsin G (Cat G) and proteinase 3 (PR 3) was
then determined Most of the compds. were found to be potent,
-dependent.

then determined Most of the compds. were found to be potent, time-dependent inhibitors of elastase, with some of the compds. exhibiting kinact/KI values as high as 4,928,300 M-l s-l. The inhibitory potency of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform was found to be influenced by both the pKa and the inherent structure of the leaving group. Proper selection of the primary specificity group was found to lead to selective inhibition of HLE over Cat G, however, those compds. that inhibited HLE also inhibited PR 3, albeit less efficiently. The predictable mode of binding of these compds.

compds.

suggests that, among closely-related serine proteases, highly selective inhibitors of a particular serine protease can be fashioned by exploiting subtle differences in their S' subsites.

17 24119-63-1p 281921-30-69 281921-33-9p 281921-31-39-29 281921-32-92 281921-42-0p 281921-45-3P 281921-39-5p 281921-42-0p 281921-45-3P 281921-46-4P 281921-52-2P 281921-54-4P 281921-65-7P 281921-91-9P RL: BBC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological)

(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis of thiadiazolidinone dioxides and isothiazolidinone dioxides

ides as serine protease inhibitors) 247179-63-1 RCAPUS 1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy]methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 300553-85-9 HCAPLUS 1,2,5-Thiediazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

REFERENCE COUNT: THIS

THERE ARE 27 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-30-6 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[4-ethyl-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiarolidin-2-yl]methyl ester [9CI] (CA INDEX NAME)

287921-33-9 HCAPLUS
Benzeneacetic acid, 4-{[(35)-5-[(2,2-dimethyl-1-oxopropoxy)methyl]-1,1-dioxido-4-oxo-3-propyl-1,2,5-thiadiazolidin-2-yl]methyl]- (9C1) (CA INDEX

NAME)

Absolute stereochemistry.

RN 287921-37-3 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[(8)]-4-(2-methylpropyl)-1,1-dioxido-3-oxo5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

287921-38-4 HCAPLUS
Benzeneacetic acid, 4-[[(1S)-5-[(2,2-dimethyl-1-oxopropoxy|methyl]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-39-5 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-42-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(benzoyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenepropanoic acid, {(48)-4-(2-mathylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-54-4 HCAPLUS
Benzeneacetic acid, [(45)-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 287921-65-7 HCAPLUS
CN Benzoic acid, 2,6-dichloro-,
[(48)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

26/921-91-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-{(acetyloxy}methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 287921-45-3 HCAPLUS
CN Benzoic acid, 2,6-dichloro-,
[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5{phenylmethyl}-1,2,5-thiadiazolidin-2-yl]methyl ester (9C1) (CA INDEX NAME)

(Continued)

287921-46-4 RCAPLUS
Benzeneacetic acid, 4-[[(35)-5-[[(2,6-dichlorobenzoyl)oxy]methyl]-3-[2-methylpropyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- [9CI]
(CA INDEX NAME)

Absolute stereochemistry.

287921-52-2 HCAPLUS

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

212331-98-1P 212331-99-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxides and isothiazolidinone

(synthesis of discrete control of the control of th

212331-99-2 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

FORMAT

THERE ARE 44 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 May 2000
ACCESSION NUMBER: 2000:324184 HCAPLUS
DOCUMENT NUMBER: 133:105000
TITLE: Solid-phase synthesis of sulfahydantoins
Althrox(5): Albericio, Pernando; Garcia, Javier; Hichelotti,
Enrique L.; Nicolas, Ernestor, Tice, Colin M.
Department of Organic Chemistry, University of
Barcelona, Barcelona, 08028, Spain
Tetrahedron Letters (2000), 41(17), 3161-3163
CODEN: TELEAY; ISSN: 0040-4039
Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

LANGUAGE:

OTHER SOURCE(S):

MENT TYPE: Journal
UAGE: English
R SOURCE(S): CASREACT 133:105000
A 5-step solid-phase synthesis of 2-unsubstituted 1,2,5-thiadiazolidin-3one 1,1-dioxides, sulfahydantoins, from Nn-Fmoc amino acids and
aromatic aldehydes is described. The key step is the base-mediated
files

asomatic aldenydes is described. The key step is the base-medifitive cleavage of a resin bound Nd-aminosulfonyl Nd-benzyl amino acid to afford the desired product. This synthesis allows the paration of a diverse library of compds. based on this heterocycle. 283587-14-49 283587-15-59 283587-16-69 283587-18-99 283587-21-3P 283587-22-4P 283587-24-69 RI: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of sulfahydantoin library) 283587-14-4 RCAPLUS 1,2,5-Thadiszolidin-3-one, (4-methoxyphenyl)methyl)-4-(phenylmethyl)-, l,-ioxide, (45)- (9CI) (CA INDEX NAME)

IT

283587-15-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{2,4-dichlorophenyl}methyl}-4{phenylmethyl}-, 1,1-dioxide, {45}- {9CI} {CA INDEX NAME}

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[{2-chlorophenyl}methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,1,1-dioxide (9CI) (CA IMDEX NAME)

283587-24-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[2(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

14 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

283587-16-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, -methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-(1-methylethyl)-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS CN 1,2,5-fhiadiazolidin-3-one, 5-[{2,3-dihydro-1,4-benzodioxin-6-y1}methy1]-4-(1-methylethy1}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

(Continued) L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR 29

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 27 Aug 1599 ACCESSION NUMBER: 1599:5316684 HCAPLUS DOCUMENT NUMBER: 131:296963 HUMBER: 1500 ACCESSION ACCESSION NUMBER: 1500 ACCESSION NUMBER: 1500 ACC ACCESSION NUMBER: 1999:536684 RCAPLUS
DOCUMENT NUMBER: 131:296963
ITITLE: Human chymase inhibitors based on the
1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold
Groutas, William C.; Schechter, Norman M.; Me, Shu;
YU, Hongyi; Huang, Peng; Tu, Juan
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic 4 Medicinal Chemistry Letters (1999),
9(15), 2199-2204
COORN BMCLES; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of compds. that utilize the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold was synthesized and shown to be highly effective
inhibitors of recombinant human skin chymase.

IT 170918-99-7 247178-61-2 247179-63-1
247179-64-2 247179-68-6 247179-66-4
247179-70-0 247179-71-2 247179-76-7
247179-70-0 247179-71-2 247179-76-7
RL: BBC (Biological activity or effector, except adverse); BSU
(Biological
Study, unclassified); PRP (Properties); BIOL (Biological study)
(human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold)
RN 170918-99-7 HCAPLUS
CN 1,2,5-thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 KCAPLUS
Benzoic acid, 4-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
CN Acetic acid, hydroxy-,
[{45}-1,1-dioxido-3-oxo-4,5-bis[phenylmethyl]-1,2,5thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 247179-66-4 HCAPLUS
CN Propanoic acid, 2-hydroxy-,
[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-67-5 HCAPLUS Enterone member 2 member 2 member 2 member 3 mem

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-63-1 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2-{(acetyloxy)methyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-64-2 HCAPLUS
Propanedioic acid, mono[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]mathyl) ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

247179-65-3 HCAPLUS

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

247179-68-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(methylsulfonyl)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-69-7 HCAPLUS
Acetic acid, [[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

247179-70-0 HCAPLUS
Propanoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

247179-71-1 HCAPLUS
Benzoic acid, 2-{[[(43)-1,1-dioxido-3-oxo-4,5-bis|phenylmethyl]-1,2,5-thiadiazolidin-2-ylmethyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-72-2 HCAPLUS
Benzoic acid, 3-[[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

25

REFERENCE COUNT: THIS

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-74-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl)-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-75-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-benzoxazoly1)thio]methyl]-4,5-bis[phenylmethyl]-1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-76-6 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4,5-bis(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 25 Aug 1999
ACCESSION NUMBER: 1999:529936 HCAPLUS
DOCUMENT NUMBER: 131:296959
TITLE: A General Inhibitor Scaffold for A General Inhibitor Scaffold for Serine Proteases

A General Inhibitor Scaffold for Serine Proteases

a (Chymo)trypsin-Like Fold: Solution-Phase
Construction and Evaluation of the First Series of
Libraries of Mechanism-Based Inhibitors
Kuang, Rongre: Epp, Jeffrey B.; Ruan, Sumeir Yu,
Hongyi: Huang, Peng; He, Shu; Tu, Juan: Schechter,
Norman M.; Turbov, Jane; Froelich, Christopher J.;
Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Journal of the American Chemical Society (1999),
121(35), 8128-8129
CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors demonstrate that the 1,2,5-thiadiazolidin-1-one 1,1 dioxide platform embodies a general motif that renders the platform capable of binding to the active site of many serine processes with a (chymo)trypsin-like fold in a predictable fashion and is amenable to the facile construction of libraries for lead identification and optimization.

If 170918-99-Pp 170919-03-6P 189124-02-5P 247178-9-9P 247178-99-Pp 247178-40-1P 247178-41-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

RE: BAC (Biological activity of effector, except activities, Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (inhibitor; general inhibitor scaffold for serine proteases with a (chymo)trypsin-like fold with solution-phase construction and

(chymo)trypsin-like fold with solution-phase construction and
evaluation
of first series of libraries of mechanism-based inhibitors)
RN 170918-99-7 HCAPLUS
1,2,5-Thiadizolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry.

RN 189124-02-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-2-(phenylmulfonyl)methyl)-4-propyl-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-39-8 HCAPLUS 1,2.5-Thiadiacrididin-3-one, 4-(4-aminobuty1)-5-(phenylmethy1)-2-((phenylmethy1)-1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 16 Mar 1999
ACCESSION NUMBER: 1999:172588 HCAPLUS
INCUMENT NUMBER: 130:209985
ITITLE: Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as serine protease inhibitors
Groutas, Milliam C.: Kwang, Rongze
Wichita State University, USA
POT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: PREDICT PROPRATION: English
FAMILY ACC. NUM. COUNT: English
PATENT INCORPARATION: 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE DATE MO 9909977 A1 19990304 W0 1998-US17406 19980821
W: AU, BR, CA, IS, JP, MX, NZ
RN: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE
US 6420401 B1 20020716 US 1997-916693 19970822
AU 9890298 A 19990316 AU 1998-90298 19980821
EP 1011668 A1 20000628 EP 1998-942192 19980821 R: DE, GB PRIORITY APPLN. INFO.: US 1997-916693 A 19970822

WO 1998-US17406

w 19980821

OTHER SOURCE(S): MARPAT 130:209985

AB Substituted 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivs. I (R1, R3 = independently H, alkyl, aryl, aralkyl, alkaryl, substituted aryl; R2 = H, alkyl, aralkyl, arlkyl, arilyl, aralkyl, aryl, aralkyl, aryladic aryl; R2 = H, alkyl, aryl, aralkyl, aryladic aryl; R2 = H, alkyl, aryl, aralkyl, amino acid side chain; R4 = H, alkyl, aryl, aralkyl, amino acid side chain; P03R82, NCO, NHCHRTGO2R10, NHCONR12R13, CO-Q, -CHR7NHW, [CHR7NHCO]rR10, [CHR7CONH]rR10, NHC; NHC; NHCHR7CO]NHIRDIG, OPN, NHPN; R5 = R1, halo; R6 = H, alkyl, aryl, aralkyl, NCO, COR3, COO1, NHCHR7CO2R11, NHZ, NHC, NHCO2R11, NHCONR14R15, O2COHZ[OCHZCH2]2OR, O-X; R = alkyl; Q1 = OR11, O2, NHIRDIS, CONSCRIPTION (CONRCHIP) (CO

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247178-40-1 KCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-5-(phenylaulfonyl)methyl]-, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS Benzoic acid, 4-[[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THIS

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) = G, H; m = 1-2; each R7 = amino acid side chain; each R8, R9 = alkyl, aryl, aralkyl, alkaryl, heterocyclyl; each R10-R15 = H, any group R8;

R16, R17 = heterocyclylalkyl; R18 = any group R8, NHR19; R19 = alkyl, aryl, aralkyl; with provisos], oligomers and combinatorial libraries contg. them, and methods of using them, are disclosed. Thus, title

contg. them, and methods of using them, are disclosed. Thus, title

II showed apparent second-order rate consts. Kinact/KI (M-ls-1) of

119,360, 27,400, and 60 for inhibition of human leukocyte elastase,
proteinase 3. and cathepsin G, resp., by in vitre assays.

220868-4-6-PP, combinatorial library derivs. 220868-8-75-TDP

, combinatorial library derivs. 220868-80-4DP, combinatorial library derivs.

220868-86-0DP, combinatorial library derivs. 220868-87-TDP

combinatorial library derivs. 220869-20-PP, combinatorial

library derivs. 220868-93-9DP, combinatorial library derivs.

220869-86-98-4DP, combinatorial library derivs. 220868-99-DP

combinatorial library derivs. 220869-05-6P

220869-06-7P 220869-07-8P 220869-10-7P

220869-18-9P 220869-19-2P 220869-20-5P

220869-18-9P 220869-19-2P 220869-20-5P

220869-18-7P 220869-31-0P 220869-31-0P

220869-38-5P 220869-31-0P 220869-31-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

iogical
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of amino acid-derived thiadiazolidinone dioxide derivs.

serine protease inhibitors)
RN 220868-74-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(4-methoxyphenyl)methyl]-,
1,1-dioxide [901] (CA INDEX NAME)

CH2C1

220868-75-7 HCAPLUS

NN Z2UBBE-79-7 MCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(3-phenoxyphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-80-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(acetyloxy)methyl1-5-{(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220868-81-5 HCAPLUS 1,2,5-Thiadizolidin-3-one, 2-[(acetyloxy)methyl]-5-[(3-phenoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220868-92-8 HCAPLUS
CN L-Phenylalanine,
4-chloro-W-[[[[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220868-93-9 HCAPLUS
CN L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl][9CI]

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-86-0 HCAPLUS
Carbamic acid, [[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3-oxo-1,2,5-thiadiarolidin-2-yl]methyl)(methylsulfonyl)-, methyl ester [9CI) (CA INDEX MAME)

220868-87-1 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-5-{(3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

RN 220868-98-4 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-99-5 HCAPLUS L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[[3-phenoxyphenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]-(9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

220869-06-7 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, phenylmethyl ester (9CI)(CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN L4

(Continued)

220869-19-2 HCAPLUS

RN 220869-19-2 HCAPLUS
CN Glycine,
N-([[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](phenylsulfonyl)amino]carbonyl)-, ethyl ester
(9CI) (CA INDEX NAME)

220869-20-5 HCAPLUS 1,2,5-Thiediarolidin-3-one, 2,2'-methylenebis[4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester [9CI) (CA

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-26-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[{(4,5-diphenyl2-2-oxazcly1)thio]methyl]-4-{2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(5-

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phonyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-30-7 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (901) (CA INDEX NAME)

220869-13-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-2-{{3-phenyl-1,2,4-oxadiazol-5-yl}thio}methyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

(Continued) ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-40-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-bentoxazoly1)thio]methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-41-0 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, u-fluoro-3-oxo-4,5-bis(phenylmethyl)-, ethyl ester, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

220869-64-7 220869-65-8
RL: RCT (Reactant), RACT (Reactant or reagent)
(preparation of amino acid-derived thiadiazolidinone dioxide derive.

serine protesse inhibitors)
220869-64-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-2-[{(5-phenyl-2-benzozzolyl)thio]methyl}-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-39-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[((5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

220869-65-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-61-4P 220869-62-5P 220869-63-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) [preparation of amino acid-derived thiadiazolidinone dioxide derivs.

serine protease inhibitors)

200869-61-4 HCAPLUS

1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dimethylethyl ester, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-62-5 RCAPLUS
1,2,5-Thiadiacolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-63-6 HCAPLUS
1,2,5-Thiadiazolidino-2-acetamide, 4-(2-methylpropyl)-3-oxo-N-(2-phenylethyl)-5-(penylmethyl)-, 1,1-dioxide, (45)- (5C1) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

15

REFERENCE COUNT: THIS

THERE ARE 15 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 02 Oct 1998
ACCESSION NUMBER: 1990:622789 HCAPLUS

DOCUMENT NUMBER: 129:289736

Kinetics of the hydrolysis of cyclic N-substituted sulfamides: 4-amino-2-cyclohexyl- and 4-amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5-chiadiazole 11,1-dioxides

AUTHOR(S): Rozas, M. F.; Svartman, E. L.; Mirifico, M. V.; Vasini, E. J.

CORPORATE SOURCE: Instituto de Investigaciones Fisicoquimicas Te6ricas

Aplicadas (INIFTA), Facultad de Ciencias Exactas,
Departamento de Quimica, Universidad Nacional de La
Plata, La Plata, 1900, Argent.
Journal of Physical Organic Chemistry (1998), 11(7),
489-694

CODEN: JPOCEE: ISSN: 0894-3230 John Wiley & Sons Ltd. Journal

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

SOURCE:

UAGE: English
The hydrolysis reactions of 4-amino-2-phenethyl- and

unit

slope is observed from pH ca 4 up to the highest exptl. pH (ca 10). The products are the corresponding new compds.: 2-mino-2-[(N-substituted-sulfamoyl)imino]acetic acid salts. The c=N bond of these compds. hydrolyres further, in a slow reaction, to the sulfamide and oxalic acid derivs. The substrates decompose to the final products without accumulation

accumulation
of the acetic acid derivs. under these exptl. conditions. A mechanism is
proposed. Rate consts. and activation parameters are given for the first
reaction step. Owing to steric effects, the reaction rate is higher for
the N-phenethyl-substituted derivative than for the
2-cyclohexyl-substituted
derivative
IT 214216-09-8, 4-Amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5thiadiazole 11,1-dioxide
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
RCT

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006.ACS on STN

ED Entered STN: 05 Aug 1998
ACCESSION NUMBER: 1998:407562 HCAPLUS
1299:216561
Potent and specific inhibition of human leukocyte elastase, cathepsin G and proteinase 3 by sulfone derivatives employing the 1,2,5-thiadiazolidin-3-one 1,1-doxide scaffold
Groutas, William C.; Kuang, Ronger; Ruan, Sumei; Epp, Jeffrey B.; Venkataraman, Radhika; Truong, Tien M. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (1998), 6(6),

SOURCE: 661-671

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd. PUBLISHER:

Journal English

DOCUMENT TYPE: LANGUAGE: GI

This paper describes the results of structure-activity relationship studies in a series of heterocyclic mechanism-based inhibitors based on the 1.2.5-thiadiazolidin-3-one 1.1-dioxide scaffold (Ir Rl = iso-Bu, benzyl; RZ = Bu, Me, benzyl; RZ (RZCOCMEA), etc.; L = SOZPh, SOZCEMEC1-4, etc.) and capable of interacting with the Sn and S'n subsites of a serine proteinase. Sulfone derivs. of I were found to be highly effective, time-dependent inhibitors of human leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3). The judicious selection of an Rl group (accommodated at the primary specificity site 51) that is based on the known substrate specificity of a target serine proteinase, was found to yield highly selective inhibitors. The presence of a benzyl group (RZ = benzyl) at the SZ subsite was found to lead to a pronounced enhancement

inhibitory potency. Furthermore, the effective use of computer graphics and modeling has led to the design of potent, water-soluble inhibitors.

results of these studies demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1-dioxide platform provides an effective means for appending

1,1-dioxide platform provides an effective means for appending recognition
elements in a well-defined vector relationship, and in fashioning highly-selective and potent inhibitors of serine proteinases.

IT 212331-98-19 212331-99-29 212332-00-8P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant) or reagent)
(1,2,5-thiadiazolidin-3-one 1,1-dioxide inhibitors of human leukocyte elastase, cathepsin G and proteinase 3)

RN 212331-98-1 MCAPLUS

2.2.3.3-39-1 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylthio)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212332-00-8 HCAPLUS
Benzeneacetic acid, 3-[[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 212331-79-8P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and
proteinase 3)
RN 212331-79-8 HCAPLUS

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry. Double bond geometry as shown.

170919-03-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-77-6 HCAPLUS
Benzoic acid, 4-[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester
[9C1] (CA INDEX NAME)

Absolute stereochemistry.

212331-78-7 HCAPLUS
Benzoic acid, 4-[{(35)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5-[(phenylsulfonyl)methyl}-1,2,5-thiadiazolidin-2-yl)methyl}- (9CI) (CA INDEX NAME)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)
Benroic acid, 3-[[(35)-3-{2-mothylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl)methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

170918-99-7P 170919-01-4P 170919-03-6P 212311-77-6P 212331-78-7P 212331-80-1P 212331-81-2P 212331-82-3P 212331-83-4P 212331-66-7P 212331-97-6P 212331-90-3P 212331-92-5P 212331-94-7P 212331-95-8P 212331-97-0P RL: BAC (Biological activity or effector, except adverse); BSU

RL: BAC (Biological activity or execut, energy execution); BIOL (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3)
RN 170918-99-7 RCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(phenylmethyl)-5-[(2E)-3-phenyl-2-propenyl)2-(phenylsulfonyl)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

212331-80-1 HCAPLUS
Benzoic acid, 3-[([35]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

212331-81-2 HCAPLUS
Benzoic acid, 2-[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
[9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-82-3 HCAPLUS Benzoic acid, 2-{((3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-83-4 HCAPLUS
CN Benzeneacetic acid, 4-{[{3S}-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5-{(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-{[(4-chlorophenyl)sulfonyl]methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-92-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[((3-phenylpropyl))]-1,1-dloxide, (45)- (5C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-94-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[3-(critlucromethyl)phenyl]sulfonyl]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-95-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(2-phenylethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[[(4-chlorophenyl]methyl]sulfonyl]methyl]-4{2-methylpropyl)-5-[phenylmethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-97-0 HCAPLUS
CN Benzeneacetic acid, 4-[[(35)-1,1-dioxido-4-oxo-3-(phenylmethyl)-5[(phenylsulfonyl)methyl)-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

```
L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Apr 1998 ACCESSION NUMBER: 1998:200895 HCAPLUS DOCUMENT NUMBER: 128:278642
                                                                                                                              128:278642
Use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent inhibitors of serine proteinases Kuang, Rongze: Venkataraman, Radhika: Ruan, Sumei: Groutas, William C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1998),
 CORPORATE SOURCE:
                                                                                                                                539-544
CODEN: BMCLEB; ISSN: 0960-894X
Elsevier Science Ltd.
Journal
 CODEN: BMCLES; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: Brglish

The attachment of a phosphate leaving group to the
1,2,5-thiadiazolidin-3-
one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds was found
to yield highly potent, time-dependent inhibitors of human leukocyte
elastase (HLE).

17 205932-85-0P 205932-87-2P 205932-88-3P
205332-83-4P
RL: BAC (Biological activity or effector, except adverse); BSU

(Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
                        logical
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and
isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent
inhibitors of serine proteinases)
205932-85-0 HCAPUUS
Phosphoric acid, dimethyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-
(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX
NAME)
```

Phosphoric acid, dibutyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phonylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

```
L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN
ED Entered STN: 30 Aug 1997
ACCESSION NUMBER: 1997:555602 HCAPLUS
                                            127:257045
        MENT NUMBER:
                                            127:237043
Competitive particle concentration fluorescence
immunoassays for measuring antidiabetic drug levels
TITLE:
in
                                             mouse plasma
                                             mouse plasma
Bright, Stuart W.; Tinsley, Frank C.; Dominianni,
Samuel J.; Schmiegel, Klaus K.; Fitch, Lora L.; Gold,
AUTHOR(S):
CORPORATE SOURCE:
```

Gerald Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA Journal of Immunological Methods (1997), 207(1), SOURCE: 23-31 CODEN: JIMMBG: ISSN: 0022-1759

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two competitive particle concentration fluorescence immunoassays were
developed
to measure blood levels of analogs of antidiabetic drugs being tested in
diabetic mics. Ligands that contained the active pharmacophores were
conjugated to PPD for immunization and to 6-phycocrythrin for use as
a tracer in the immunoassays. Approx. 90% of 262 compds. assayed were
detectable at less than 120 nM in plasma which was well below the

therapeutic level of 1 μ M for lowering blood glucose. These data were used to define the bioavailability of test compds. and assist in

decisions
of constructing active analogs. Of addnl. interest, we noted
crossreactivity of one monoclonel antibody for 3 different compound

that are all known to bind with varying affinities to peroxisome proliferator-activated receptors. 196079-43-3 RE: ANT (Analyte); ANST (Analytical study) (competitive particle concentration fluorescence immunoassays for

measuring
antidiabetic drug levels in mouse plasma)
RN 196079-43-3 KCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[2-(2-phenyl-4-oxazolyl)ethoxy]phenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR 13

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

205932-88-3 HCAPLUS Phosphoric acid, (4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl bis(phenylmethyl) ester (9CI) (CA INDEX

205932-89-4 HCAPLUS
Phosphoric acid, [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-chiadiazolidin-2-yllmethyl diphenyl ester (9C1) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Apr 1997 ACCESSION NUMBER: 1997:226843 HCAPLUS DOCUMENT NUMBER: 126:287581 TITLE:

Structure-Based Design of a General Class of Mechanism-Based Inhibitors of the Serine Proteinases Employing a Novel Amino Acid-Derived Heterocyclic Scaffold Scaffold
Groutas, William C.; Kuang, Rongze; Venkataraman,
Radhika; Epp, Jeffrey B.; Ruan, Sumei; Prakash, Om
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Biochemistry (1997), 36(16), 4739-4750
CODEN: BICHAW; ISSN: 0006-2960
American Chemical Society
Journal AUTHOR (5):

CORPORATE SOURCE:

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We describe in this paper the structure-based design of a general class

heterocyclic mechanism-based inhibitors of the serine proteinases that embody in their structure a novel peptidomimetic scaffold (1,2,5-thiadiazolidin-3-one 1,1-dioxide). Sulfone derivs of this class were time-dependent, potent, and highly efficient irreversible inhibitors of human leukocyte elastase, cathepsin G, and proteinase 3. The partition ratios for a select number of inhibitors were found to range between 0 and 1.

and 1.

We furthermore demonstrate that these inhibitors exhibit remarkable

enzyme
selectivity that is dictated by the nature of the Pl residue and is
consistent with the known substrate specificity reported for these
enzymes. Thus, inhibitors with small hydrophobic side chains were
effective inhibitors of elastase, those with aromatic side chains of
cathepsin G, and those with a basic side chain of bovine trypsin. Taken
together, the findings cited herein reveal the emergence of a general
class of stable mechanism-based inhibitors of the serime proteinases
which

which

can be readily synthesized using amino acid precursors. Biochem. and
high-field NMR studies show that the interaction of this class of
inhibitors with a serine proteinase results in the formation of a stable
acyl complex(es) and the release of benzenesulfinate, formaldehyde, and a
low mol. weight heterocycle. The data are consistent with initial
formation
of a Michaelis-Menten complex, acylation of Ser195, and tandem loss of
the

leaving group. The initial HLE-inhibitor complex reacts with water generating formaldehyde and a stable HLE-inhibitor complex. Whether the initial HLE-inhibitor complex also reacts with His57 to form a third complex is not known at this point. The desirable salient parameters associated with this class of inhibitors, including the expeditious generation of structurally diverse libraries of inhibitors based on I, suggest that this class of mechanism-based inhibitors is of general applicability and can be used in the development of inhibitors of human and viral serime proteinses of clin. relevance.

170918-99-79 170919-01-69 189124-00-99
RL: BRC (Biological activity or effector, except adverse); BSU logical

RI: BAC (Biological activity or effector, except adverse; associations); BIOL (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and structure activity relations of mechanism-based inhibitors

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) of human leukocyte serine proteinases employing a novel amino acid-derived heterocyclic scaffold)
170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-(phenylsulfonylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylmylfonyl)methyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

189124-00-3 HCAPLUS
1,2,5-Thiadizolidin-3-one, 4-ethyl-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylnethyl)-2-([phenylsulfonyl)methyl]-4propyl-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-04-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{1-methylethyl}-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-06-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-butyl-5-(phenylmethyl)-2-

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 01 Dec 1995
ACCESSION NUMBER: 1995:954574 HCAPLUS
123:340140
Novel serine protease inhibitors: derivatives of isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide Groutas, William C.

PATENT ASSIGNEE(S): Wichta State University, USA
POCUMENT TYPE: PATENT ASPI., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent LANGUAGE: English
PAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.						KIND DATE				APPLICATION NO.						DATE		
						A1 19950713			WO 1995-US236						19950103				
		W:	AM,	AT,	ΑU,	BB,	BG,	BR,	BY,	CA,	CH	, CN,	CZ,	DE,	DK,	ES,	FI,	GB,	
			GE.	HU.	JP,	KE,	KG,	K₽,	KR,	ΚZ,	LK	, LT,	LU,	LV,	MD,	MG,	MN,	MW.	
			NL,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE	, SI,	SK,	ΤJ,	TT,	UA,	UZ,	VN	
		RW:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IE,	IT,	LU,	MC,	NL,	PT,	SE	
	us	5550	139			Α		1996	0827		ŲS	1994-	1773	52		1	9940	103	
	CA	2179	913			A1		1995	0713		CA	1995-	2179	913		1	9950	103	
	AU	9515	998			A		1995	0801		ΑU	1995-	1599	В		1	9950	103	
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											EΡ	1995-	9080	03		1	9950	103	
		7393																	
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IE,	IT,	LI,	LU,	MC,	NL,	PT,	
SE																			
	JP	0950	9922			T		1997	1007			1995-							
	AT	2159	38			T T		2002	0415		AT	1995-	9080	03		1	9950	103	
	NZ	3297						2001	0223		NZ	1998-	3297	66		1	9980	216	
PRIO	RIT	APP	LN.	INFO	. :						US	1994-	1773	52		A 1	9940	103	
											WO	1995-	US23	6		w 1	9950	103	

OTHER SOURCE(S): MARPAT 123:340140

Various isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide derivs., e.g. I (X = CN2, (un)substituted NH; Rl = H, alkyl, (un)substituted benzyl, indolylalkyl, etc.; Y = non-steroidal antiinflammatory residue, H, protected amino acid, acyloxy, etc.), and their use to reduce or inhibit the activity of serine proteases, are claimed. The compds. are useful as anti-inflammatory and anti-necastatic agents. For example, 4-benzylisothiazolidin-3-one 1,1-dioxide underwent

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) N-alkylation with ClCH25Ph and Et3N in MeCN, followed by S-oxidn. with m-clCGH4C(0)00M in CH2C12 [901), to give title compd. II. In an in vitro assay, II had an apparent 2nd-order inactivation rate const. (kobs/[I]

M-1
s-1) of 960 against cathepsin G. A variety of compds. were prepd. and/or tested against cathepsin G, human leukocyte elastase, and/or protesinase-3.
17 170919-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-16-1 RCRPLUS
CN 1.2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-(3-phenyl-2-propenyl)-2-(phenylthio)methyl)-, 1,1-dioxide, [5-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 170919-15-0P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological)
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-15-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4,5-bls(phonylenthyl)-2-[(phenylthio)methyl]-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

1.4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 170919-03-6 170919-21-8 170919-22-9
RI: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): THU (Therapeutic use): BIOL (Biological study);

USES (Uses)

(Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-03-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-21-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylsulfonyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

BN 170919-22-9 HCAPLUS

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) IT 153044-45-2P 170918-99-7P 170919-01-4P
R1: BAC (Biological activity or effector, except adverse); BSU
(Biological study); PREP (Preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as /s. as serine protease inhibitors)
153044-45-2 MCAPUUS
1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-[(2E)-3-phenyl-2-propenyl]-2-{(phenylmethyl)-bethyl}-, 1,1-dioxide, (45)- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:124451 HCAPLUS
DOCUMENT NUMBER: 120:124451
TITLE: Substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides:
a new class of potential mechanism-based inhibitors

AUTHOR(5):

human leukocyte elastase and cathepsin G Groutas, William C.; Kuang, Rongze; Venkataraman, Radhika Dep. Chem., Wichita State Univ., Wichita, KS, 67260, USA Biochemical and Biophysical Research Communications (1994), 198(1), 341-9 CODEN: BBRCA9; ISSN: 0006-291X Journal English CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: GI

A series of substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides (I, R = benzyl; R1 = H. Me, benzyl, CH2CO2-tert-Bu or CH2CO2-benzyl) was prepd, and their in vitro inhibitory activity toward human leukocyte elastase

and

cathepsin G was investigated. These compds. inactivated the 2 enzymes efficiently and in a time-dependent fashion.

IT 153044-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and human leukocyte elastase and cathepsin G inhibition by)
RN 153044-45-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Jan 1991
ACCESSION NUMBER: 1991:23940 HCAPLUS DOCUMENT NUMBER: 114:23940
TITLE: Intra- and intermolecular a-sul

114:23940
Intra- and intermolecular q-sulfamidoalkylation reactions
Lem, Chai Ho: Kohn, Harold
Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA AUTHOR(S): CORPORATE SOURCE:

USA
Journal of Organic Chemistry (1990), 55(25), 6098-104
CODEN: JOCKAH: ISSN: 0022-3263
Journal
English
CASRERCT 114:23940 SOURCE:

DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE(S):

CO₂Et

The utility of α -sulfamidoalkylation processes for the generation of sulfamides has been examined. Both intra- and intermol. α -sulfamidoalkylation transformations were observed to proceed in moderate

good yields. The generality of these processes has been demonstrated using N.N'-di(aryl-substituted)sulfanides, and the utility of these reactions was examined for the preparation of cyclic sulfamides of novel structure. Thus, reaction of PhCHENNSOZNHZ with ECOZCCH(OEL)2 in the presence of CF3COZH gave 74% dichiatetracocinedicarboxylate tetraoxide I, whereas reaction of 3-MeOCEH4CHZNHSOZNHZ with ECOZCCH(OEL)2 in CF3COZH followed by methylation gave benrothiadizatepinecarboxylate tetraoxide I, the crystal structures of I and II were determined 130670-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or resgent)
(preparation and cyclization of) 130670-00-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-hydroxy-5-(2-phenylethyl)-, 1,1-dioxide, monosodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

(Continued)

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                 ADISCTI Reloaded and Enhanced
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                 truncation
                 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS
     8
         SEP 25
                 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
         SEP 25
NEWS
     9
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10
         SEP 25
                 CEABA-VTB classification code fields reloaded with new
         SEP 28
NEWS 11
                 classification scheme
                 LOGOFF HOLD duration extended to 120 minutes
         OCT 19
NEWS 12
                 E-mail format enhanced
NEWS 13
         OCT 19
                 Option to turn off MARPAT highlighting enhancements available
NEWS 14
         OCT 23
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 15
         OCT 23
                 multiple databases
                 The Derwent World Patents Index suite of databases on STN
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         OCT 23
                 has been enhanced and reloaded
                 CHEMLIST enhanced with new search and display field
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         OCT 30
         NOV 03
                 JAPIO enhanced with IPC 8 features and functionality
NEWS 18
                 CA/CAplus F-Term thesaurus enhanced
         NOV 10
NEWS 19
                 STN Express with Discover! free maintenance release Version
NEWS 20
         NOV 10
                 8.01c now available
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 21
         NOV 20
                 additional databases
                 CA/CAplus to MARPAT accession number crossover limit increased
NEWS 22
         NOV 20
                 to 50,000
                 CAS REGISTRY updated with new ambiguity codes
         DEC 01
NEWS 23
         DEC 11
                 CAS REGISTRY chemical nomenclature enhanced
NEWS 24
                 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25
         DEC 14
                 GBFULL and FRFULL enhanced with IPC 8 features and
         DEC 14
NEWS 26
                 functionality
                 CA/CAplus pre-1967 chemical substance index entries enhanced:
         DEC 18
NEWS 27
                 with preparation role
                 CA/CAplus patent kind codes updated
         DEC 18
NEWS 28
         DEC 18
                 MARPAT to CA/CAplus accession number crossover limit increased
NEWS 29
                 to 50,000
         DEC 18 MEDLINE updated in preparation for 2007 reload
NEWS 30
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AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10510026RTRexpand.str

chain nodes :
7 9 18 19 22 23
ring nodes :
1 2 3 4 5 10 11 12 13 14 15
chain bonds :
1-22 1-23 2-7 4-18 4-19 5-9 9-10
ring bonds :
1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-2 1-5 1-22 1-23 2-3 2-7 3-4 4-5 4-18 4-19 5-9
exact bonds :
9-10
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15

G1:H,CH3

G2:0,S

G3:0, S, N

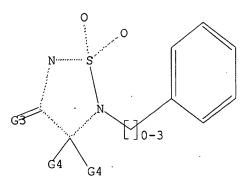
G4:H,CH3 -

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0, S

G3 O, S, N

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s 11SAMPLE SEARCH INITIATED 14:03:30 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -68 TO ITERATE

50 ANSWERS 100.0% PROCESSED 68 ITERATIONS

SEARCH TIME: 00.00.01

COMPLETE FULL FILE PROJECTIONS: ONLINE

COMPLETE BATCH

PROJECTED ITERATIONS: 866 TO 1854

PROJECTED ANSWERS: 576 TO 1424

50 SEA SSS SAM L1 L2 ·

=> s l1 full FULL SEARCH INITIATED 14:03:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -1124 TO ITERATE

766 ANSWERS 1124 ITERATIONS 100.0% PROCESSED

SEARCH TIME: 00.00.01

L3 766 SEA SSS FUL L1

=> fil hcaplus TOTAL SINCE FILE COST IN U.S. DOLLARS ENTRY SESSION 166.94 167.15 FULL ESTIMATED COST

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FILE COVERS 1907 - 21 Dec 2006 VOL 145 ISS 26 FILE LAST UPDATED: 20 Dec 2006 (20061220/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 33 L3

 \Rightarrow d ed ibib abs hitstr 1-33

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 03 Aug 2006 ACCESSION NUMBER: 2006:765251 HCAPLUS

DOCUMENT NUMBER:

Note that the second of the protein kinase activation state for treatment of the protein kinase activation state for treatment of inflammation and hyperproliferative diseases Flynn, Daniel L.; Petillo, Feter A. becipher Pharmaceuticals, LLC, USA PCT Int. Appl., 305pp.
CODEN: PIXXD2
Patent
English
2

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

INVENTOR(S):

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WG 2006081034 A2 20060803 WO 2005-U347597 20051223
WG 2006081034 A3 20061123
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DX, DM, DZ, EC, EZ, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, MM, NN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, NN, MM, MX, M2, NA, NG, NI, NO, NZ, OM, FC, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RWI AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BM, GH, CM, KE, LS, MW, MZ, NA, SD, KS, ZZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN: INFO::

OTHER SOUPCETER:

(Continued)

OTHER SOURCE(S):

MARPAT 145:211037

Novel compds. and methods of using those compds. for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and diseases characterized by hypervascularization are provided. In a preferred

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-37-4 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-[3-{{(3R)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}phenyl}-1H-pyrazol-5-yl}-N'-1-naphthalenyl- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

872171-57-8 HCAPLUS
2-Naphthalenecarboxamide, N-[3-[1,1-dimethylethyl]-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) embodiment, the compds. of the invention modulate the activation state of p38 kinase protein, b1 kinase protein, b2 kinase protein, b2 kinase protein, b2 kinase protein. D2 kinase protein. The compds. of the invention I have general formula (R1-(X))1m-A-NH-L-NH-D-(E)q-(Y)t-Q wherein R1 = aryl, heteroaryl, and heterocyclyl; X and Y = individually Q, S, alkynyl, alkenyl, etc.; A = an arom., monocycloheterocyclic, or bicycloheterocyclic ring; D = Ph or a 5-6-membered heterocyclic ring; E = Ph, pyridinyl, or pyrimidinyl; L = -C(O) - or -S(O)2-7, jm,q,t = 0-1; and Q = a substituted ring or ring system. Over 500 compds. were prepd. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester provided the propionate, which was subsequently converted to the hydrazine. Reaction of the hydrazine with 4.4-dimethyl-3-oxopentamenitrile afforded M8

3-(3-text-butyl-5-amino-IH-pyrazole-1-yl)henyl]propionate. which was coupled with 1-naphthyl isocyanate and reduced to provide ures II. In a competition assay with SKF 86002 as a fluorescent probe, II inhibited p38 MAP kinase with ICSO of

872171-35-2P, 1+[5-tert-Butyl-2-[3-[[(5)-3-methyl-1,1,4-trioxo-

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)ures 872171-37-4P, 1-[5-tert-Butyl-2-[3-]-[(RP-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)ures 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methy1]pheny1]-2H-pyrazol-3-y1]-3-(naphthalen-1-y1)urea 872171-63-6P, 1-[5-tert-Buty1-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrazol-3-y1]3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiarolidin-2-yl)methyl]phenyl]-2H-pyrarol-3-yl]-3-(4-methoxynaphthalen-1-yl)urea RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(p38 kinase inhibitor; preparation of pyrazolyl aryl ureas as

(p38 kinase inhibitor; preparetion v. p; protein kinase activation state for treatment of inflammation and hyperproliferative diseases)

RN 872171-35-2 RAPBUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-[((3S)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(SCI) (CA INDEX NAME)

872171-63-6 HCAPLUS
Urea, N-{4-chloropheny1}-N'-{3-{1,1-dimethylethyl}-1-{3-{(1,1-dioxido-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl}-1H-pyrazol-5-yl}- (9CI)
INDEX NAME)

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-39-6 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[[5-{(4-methoxyphenyl)methyl]-1,1-

872171-49-0 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl}-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-{5-tert-Butyl-2-{3-[{5-(4-methoxybenzyl)-{R})-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2R-pyrazol-3-yl]-3-(naphthalen-1-yl]urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-[[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases)
RN 872171-36-3 HCAPLUS
CN Urea. N-[3-(1,1-dimethylethyl)-1-[3-[[(3R)-5-((4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 28 Jul 2006
ACCESSION NUMBER: 2006:739358 HCAPLUS
DOCUMENT NUMBER: 145:377543
TITLE: 15othiazolidinone heterocycles as inhibitors of protein tyrosine phosphatases: Synthesis and structure-activity relationships of a peptide

scaffold AUTHOR(S):

Yue, Eddy W.; Wayland, Brian; Douty, Brent; Crawley, Matthew L.; McLaughlin, Erin; Takvorlan, Amy; Wasserman, Zelda; Bower, Michael J.; Wei, Minr Li, Yanlong; Ala, Paul J.; Gonneville, Lucie: Wynn, Richard; Burn, Timothy C.; Liu, Phillip C. C.; Combs, Andrew P. Discovery Chemistry, Experimental Station, Incyte Corporation, Wilmington, DE, 19880, USA Bioorganic & Medicinal Chemistry (2006), 14(17), 5833-5849

CORPORATE SOURCE: SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsewier B.V. Journal English

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

Oxo- and trioxo-substituted isothiazolidinylphenylalanines are prepared

tyrosine mimetics by Suzuki coupling reactions of chloroisothiazolidinones

chloroisothiazolidinones
and chlorodioxoisothiazolidinones with N-Boc-4-borono-L-phenylalanine
derivs.; the isothiazolidinylphenylalanines (with or without subsequent
hydrogenation) are incorporated into dipeptides prepared as human protein
tyrosine phosphatase 1B (PTPIB) inhibitors such as I. of the compds.
tested, I is the most potent inhibitor of PTPIB with an IC50 value of 40
nM; the corresponding mixture of isothiazolidinone diastereomer inhibits
PTPIB with an IC50 value of 80 nM, and the separated

(R)-isothiazolidinone
diastereomer inhibits PTBIB with an IC50 value of 15.5 µM; the related
dipeptides prepared inhibit PTPIB less potently than either I or the
mixture

of isothiazolidine diastereomers containing I. Crystal structures of a

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-21-8 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(3CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-23-0 HCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI). (CA INDEX NAME)

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 Acs on STN (Continued) dioxochiazolidinone-substituted dipeptide and a dioxoiochiazolinone-substituted dipeptide bound to PTP1B are detd. by X-ray crystallog.; the low energy conformation found by ab initio calcns. for the satd. heterocycle more closely approaches the conformation obtained upon inc. T.4

heterocycle more Causary - probinding
to PTP1B than that of the unsatd, heterocycle.

IT 850315-22-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(preparation of isothiazolone- and dioxoisothiazolone-substituted
phenylelanine-containing dipeptide amides and their activities as
human

n PTP1B inhibitors) 850315-22-9 HCAPLUS L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl}-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-20-7P 850315-21-8P 850315-23-0P 910606-95-0P 910606-97-2P REL: RCT (Reactant): SPM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of isothiazolone- and dioxoisothiazolone-substituted phenylalanine-containing dipeptide amides and their activities as

n
PTP1B inhibitors)

850315-20-7 HCAPLUS
Carbanic acid, [(15)-1-[[4-[1,1-dioxido-4-oxo-5-(phenylmethyl]-1,2,5-thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

910606-95-0 HCAPLUS Benzenepropanamide, q-amino-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (qS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 910606-94-9 CMF C23 H30 N4 O4 S

Absolute stereochemistry.

2 CM CRN 76-05-1 CMF C2 H F3 02

(Continued) ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

910606-97-2 HCAPLUS
L-Phenylelaninamide,
enylelanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiarolidin-2-yl]-N-pentyl-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CRN 910606-96-1 CMF C32 H39 N5 O5 S

Absolute stereochemistry.

2 СМ

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: THIS

THERE ARE 39 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued)

FORMAT

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

AB Title compds. (RIXj)mA(NH)pLn(NH)pDEqYtQ [I; wherein R1 = {un}substituted (hetero)aryl; X, Y = independently O, S, NR6, NR65O2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene, O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h

1-4; A = (un)substituted aryl, hetero(bi)cyclyl; D = (un)substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; E = (un)substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2;

m, n, p, q, t = independently 0, 1, Q = (un)substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions]

prepared as p38 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p38 kinase protein comprises the step of contacting the a-C helix, the a-D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation

are not claimed, prepns. and/or characterization data for .apprx.150 examples of

and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester using 10% Pd/C in EtOH provided

propionate, which was treated with NaNO2 in the presence of 6N HCl and Sncl2*2R2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-(3-(3-tert-butyl-3-amino-1H-pyrazole-1-yl)phenyl)propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction

LiOH in THF/MeOH/H2O provided the urea II: In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase

[1, 2, 5] thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3- (naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-[[(R]-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3- (naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyracol-5-yl]-2-naphthalenscarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 29 Dec 2005 ACCESSION NUMBER: 2005:1346235 HCAPLUS DOCUMENT NUMBER: 144:88279 H4:88279 Preparation of 1-pyrazoly1-3-ph

Preparation of 1-pyrazolyl-3-phenylurea p38 MAP

inhibitors as antiinflammatory medicaments Flynn, Daniel L., Petillo, Peter A. USA $\,$ INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S. Ser. No. 746,460.
CODEN: USXXCO
Patent

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DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT	INFOR	MATT	UN:														
PA	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D.	ATE	
	-											-					
US	2005	2882	86		A1		2005	1229		US 2	004-	8863	29		2	0040	706
US	2004	1809	06		A1 20040916					US 2	003-		20031224				
US	7144	911			B2 20061205												
WO	WO 2006014290						2006	0209		WO 2	005-1	US23	100		2	3050	630
	WO 2006014290																
	W:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	ВĠ,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN.	co,	CR,	ςυ,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE.	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	ΚZ,
		LC.	LK.	LR,	LS,	LT.	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,
							PG,										
							TN.										
			ZM.										_				
	RW:	AT,	BE.	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,
		IS,	IT.	LT.	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,
							GQ,										
		KE.	LS.	MW.	MZ.	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,	KG,
					TJ,												
PRIORIT	Y APP	LN.	INFO	. :						US 2	003-	7464	60		A2 2	0031	224
										US 2	002-	4373	04P		₽ 2	0021	231
										US 2	002-	4374	03 B			0021	231
										05 2	002-	43/4	USP			0021	231
										US 2	002-	4374	15P		P 2	0021	231
										US 2	002-	4374	87P		P 2	0021	231

US 2003-463804P

IIS 2004-886329

P 20030418

A 20040706

OTHER SOURCE(S):

MARPAT 144:88279

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl)-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-{4-methoxynaphthalen-1-yl}urea RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(p38 kinase inhibitor; prepn. of (pyrazolyl)(phenyl)urea p38 kinase inhibitors as antiinflammatory agents)

872171-35-2 HCAPLUS

Urea, N-[3-(1,1-dimethylethyl)-1-[3-[{(3S)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-37-4 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[{(3R}-3-methyl-1,1-dioxido-4-oxo-1,2,5-chidaizolidin-2-yl]methyl]phenyl]-H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-57-8 HCAPLUS

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
2-Maphthalenecarboxamide, N-[3-(1,1-dipathylethyl)-1-[3-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (SCI) (CINDEX NAME)

872171-62-5 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-{3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolididi-2-yl)methyl)phenyl}-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9CI) (CA INDEX NAME)

872171-63-6 HCAPLUS
Urea, N-{4-chlorophenyl}-N'-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-(5-tert-Butyl-2-[3-[(5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl]urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-[4-fluorophenyl]urea 872171-49-8P, 1-[5-tert-Butyl-2-[3-[[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or respent) (preparation of (pyrazolyl) (phenyl)urea p38 kinase inhibitors as antinflammatory agents)
RN 872171-36-3 HCAPLUS
CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-[[(3R)-5-[(4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-39-6 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[[5-[(4-methoxyphenyl)methyl]-1,1-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'- (4-fluorophenyl)- (9CI) (CA INDEX NAME)

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L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Aug 2005 ACCESSION NUMBER: 2005:904352 HCAPLUS DOCUMENT NUMBER: 143:248386

DOCUMENT NUMBER: TITLE:

143:248386
Preparation of substituted arole derivatives for treating diseases mediated by PTPase activity Mjalli, Adnam M. M.; Polisetti, Dharma R.; Subramanian, Govindan; Quada, James C.; Adrimilli, Murty N.; Yarragunta, Ravindra R.; Andrews, Robert INVENTOR(S):

c.; Xie, Rongyuan USA

PATENT ASSIGNEE(S): SOURCE:

U.S. Pat. Appl. Publ., 204 pp. CODEN: USXXCO

Patent English DOCUMENT TYPE: LANGUAGE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PAT	ENT I	NO.			KIN	D	DATE									ATE			
	US 2005187277					A1		20050825			US 2	005-	5649		2	0050	211			
	ΑU	AU 2005214349				Al		2005	0901		AU 2	005-	2143	49		20050211				
	CA 2551909					A 1		2005	0901		CA 2	005-	2551	909		20050211				
	WO 2005080346																			
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			HR,	LV,	MK,	YU														
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WO 2005-US4590 W 20050211

OTHER SOURCE(S):

MARPAT 143:248386

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

The title compds. I $\{a, b = 0-2; W = 0, S, NR2 \text{ (wherein R2 = alkyl)},$

):
R1 = H, halo, CN, etc.; L1 = a direct bond, (un)substituted NHCO, NHSO2, etc.; Ar1 = (un)substituted (hetero)aryl, fused cycloalkylaryl, etc.; Ar2 = (un)substituted (hetero)arylene, fused arylcycloalkylene, etc.; L2 = CH2, O, alkylene, etc.; build can be useful as inhibitors of protein tyrosine phosphatases and thus can be useful for the management, treatment, control, or the adjunct treatment of diseases mediated by PTPase activity such as type I diabetes and type II diabetes, were

treatment, control, or the adjunct treatment of diseases mediated by PTPase activity such as type I diabetes and type II diabetes, were prepared

Thus, treating
4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1H-imidazole with Me bromacetate followed by ester hydrolysis afforded 56% [4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1H-imidazol-1-yl]acetic acid. The representative compds. I were tested for inhibition of PTP-1B. In general, the exemplified compds. I may inhibit PTP-1B with ICSO of less than 20 µM. The pharmaceutical compns. comprising the compds. I, and their use in treating human or animal disorders are also disclosed.

1861243-91-8P 863245-57-2P 863245-74-3P
863243-91-8P 863245-57-2P 863245-74-3P
863243-91-8P RL PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of substituted azole derivs. for treating diseases mediated by

PTPsase activity)
RN 863243-91-8 HCAPLUS

1,25-Thiadizolidin-3-one, 5-{4-{4-(2,4-dichlorophenyl)-2-{(1E)-2-{3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4, 4-dimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-57-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyi])-2-[(1E)-2-[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Double bond geometry as shown.

863245-74-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-H-imidarol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-05-3 HCAPLUS Benzoic acid, $4-[4-(2,4-dichloropheny1)-2-[\{1E\}-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethenyl]-1H-imidazol-1-y1]methyl]-, methyl ester (9CI) (CA INDEX NAME)$

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-80-5P 863243-92-9P 863243-93-0P
863244-06-6P 863244-07-9P 863244-08-7P
863244-13-7P 863244-77-P 863244-08-0P
863244-13-7P 863244-77-P 863244-51-3P
863244-51-7P 863244-53-5P 863245-51-3P
863244-52-4P 863244-53-5P 863245-52-4P
863245-60-7P 863245-80-3P 863245-59-4P
863245-60-7P 863245-61-PP 863245-61-PP
863245-60-PP 863245-64-PP 863245-69-PP
863245-60-PP 863245-64-PP 863245-69-PP
863245-70-4P 863245-71-0P 863245-72-1P
863245-73-4P 863245-71-0P 863245-72-1P
863245-73-4P 863245-71-0P 863245-72-1P
863245-10-0P 863245-71-0P 863245-72-1P
863245-10-0P 863245-71-1P 863245-72-1P
863245-10-0P 863245-71-1P 863245-72-1P
863246-10-0P 863245-71-1P 863245-72-1P
863246-10-0P 863245-71-1P 863246-10-5P
863246-10-0P 863246-11-1P 863246-16-6P
863287-03-0P
RL: PAC (Pharmacological activity); SPN (Synthatic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(preparation of substituted azole derivs. for treating diseases mediated by extinctly)
RN 863243-80-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

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863243-94-1 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[4-[(4-(2-chlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-92-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-2,4,4-trimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863243-93-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-phenyl-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863243-95-2 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 5-[4-[[4-{4-chloropheny1}]-2-[(1E)-2-[3'-(trifluoromethyl)]1,1'-bipheny1]-4-y1]etheny1}-1H-imidazol-1-y1]methy1]pheny1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-05-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-06-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)]1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-07-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (methylsulfonyl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazol-1-yl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-47-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(3-(trifluoromethyl)phenyl]methyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-51-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-(2-[4-(trifluoromethyl)phenyl]-1H-imidazol-1-yl]methyl]phenyl]-,

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

RN 863244-08-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-{2-chloro-4-fluorophenyl}-2-[(1E)-2[3'-(trifluoromethyl)][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-13-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[[3'-

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-52-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[[4-[2,4-dichlorophenyl]-2-[2-[2-fluoro-4{trifluoromethyl})phenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 863244-53-5 HCAPLUS '1,2,5-Thiadiarolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[2-[3'-(trifluoromethoxy|[1,1'-biphenyl]-4-yl]ethyl]-1H-imidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-25-4 HCAPLUS
CN Benroic acid,
4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-56-1 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-[(1E]-2-(3'-chloro[1,1'-biphenyl]-4-y])ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-60-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1-

methylethoxy) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-[(1E];2-[3],5]-bis[trif][uoromethyl][1,1]-bis[phenyl]-4-ylethenyl]-4-[2,4-dichlorophenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-58-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(2'-fluoro-5'-propoxy[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

863245-59-4 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN y1]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-62-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichloropheny1)-2-{(1E)-2-[4'-(1,1-dimethylethyl)[1,1'-bipheny1]-4-yl]etheny1]-1H-imidazol-1-yl]methyl]pheny1]- 1,1-dioxide (9CI) (CA INDEX NAME)

bond geometry as shown.

863245-63-0 HCAPLUS
1,2,5-Thiaddarolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(1,1-dimethylethyl)-5'-methyl[1,1'-biphenyl]-4-yl]ethenyl]-H-imidarol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-64-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-{[2-{[1E}-2-[4-(5-chloro-2-thienyl)phenyl]-lethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-66-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-([2-[(1E)-2-[4-(5-acetyl-2-thienyl)phenyl])-th-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-69-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(4,4,4-trifluorobucoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-70-9 HCAPLUS CN 1,2,5-Thiadiezolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-

fluoro-4'-(4,4,4-trifluorobutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazoll-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-67-4 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 5-{4-[{4-(2,4-dichlorophenyl)-2-{(1E)-2-[2'-fluoromethyl)[1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-68-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(3,3-dimethylbutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

14 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (C

RN 863245-71-0 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl]-4-fluoro[1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-72-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]2-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-78-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-{2,4-dichlorophenyl}-2-{(1E)-2-{4-(4,4,4-trifilorobutoxy)phenyl}-th-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(trifluoromethyl)phenoxy)phenyl|ethenyl|-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[{4-(2,4-dichlorophenyl)-2-{(1E)-2-{3'-(methylsulfonyl)}[1,1'-biphenyl]-4-yl]ethenyl}-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-04-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[(1E)-2-[4-(2,4-dichlorophenyl)-1-ethyl1H-imidazol-2-yl]ethenyl]phenyl]-, 1,1-dioxide (9CI) (CA IMDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-80-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-{{4-{2,4-dichlorophenyl}-2-{{1E}-2-{4-{4-

(1,1-dimethylethyl)phenoxy]phenyl]ethenyl]-H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-82-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichlorophenyl)-2-[(1E)-2-[4-[4-

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 863246-06-4 HCAPLUS

RN Benzoic acid, 4-[{4-(2,4-dichlorophenyl)-2-[{1E}]-2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]- (9CI)
(CA INDEX NAME)

Double bond geometry as shown.

RN 863246-09-7 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-10-0 HCAPLUS
CArbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1-2,5-thiadiazolidin-2-yl)phenyl]=nthyl]-1H-imidazol-2yl]ethenyl][1,1'-biphenyl]-3-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Double bond geometry as shown.

RN 863246-13-3 HCAPLUS.
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-((1E)-2-(4-phenoxyphenyl)]-thimidazol-1-yl]methyl]phenyl]-, 1,1-dioxide

(9CI)
(CA INDEX NAME)

Double bond geometry as shown.

RN 863246-15-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-{[4-{2,4-dichlorophenyl}-2-{(1E)-2-{3'-

(trifluoromethyl){1,1'-biphenyl}-4-yl]ethenyl}-1H-imidazol-1-yl]methyl}-2methylphenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863246-11-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(1-

methylethyl) {1,1'-biphenyl}-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl}, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-12-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-((1E)-2-(3'-methyl[1,1'-biphenyl]-4-yl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9Cl) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 863246-16-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-propyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863287-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,6-dichlorophenyl)-2-{(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-H-inidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 863247-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
mediated by
PTPase activity)
RN 863247-41-0 HCAPLUS
Benzoic acid,
4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-, methyl ester (SCI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-89-9 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

692764-94-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

852835-44-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methylphenyl)-, 1,1-dioxide (9CI) (CA

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 May 2005
ACCESSION NUMBER: 2005:378875 HCAPLUS
DOCUMENT NUMBER: 143:19267
TITLE: Structure-based design of protein tyrosine phosphatase-1B inhibitors
AUTHOR(S): Black, Emmas Breed, Jason; Breeze, Alexander L.; Embrey, Kevin; Garcia, Robert: Gero, Thomas W.; Godfrey, Linds; Kenny, Peter W.; Morley, Andrew D.; Minshull, Claire A.; Pannifer, Andrew D.; Reed, Jon; Rees, Amandas; Russell, Daniel J.; Toader, Dorin; Tucker, Julie

CORPORATE SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(10), 2503-2507
CODEN: BMCLES; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 143:19267
AB Using structure-based design, a new class of inhibitors of protein tyrosine phosphatase-1B (PTPIB) has been identified, which incorporate the 1,2,5-thiadiazolidin-3-one-1,1-dioxide template.

1,2,5-thiadiazolidin-3-one-1,1-dioxide template.
692765-80-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-based design of protein tyrosine phosphatase-1B inhibitors)
692765-80-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-44-6P 692764-89-9P 692764-94-6P 852835-44-0P 852835-45-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (structure-based design of protein tyrosine phosphatase-1B inhibitors) 612530-44-6 HCAPLUS (1230-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852835-45-1 HCAPLUS
1,2,5-Thiadiatolidin-3-one, 5-(2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 22 CITED REFERENCES AVAILABLE FOR

FORMAT

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2005
ACCESSION NUMBER: 2005:347030 HCAPLUS
DOCUMENT NUMBER: 142:411350

INVENTOR(S): Combs, Andrew P.: Yue, Eddy Wai Tsun, Bower, Michael
Jason; Zhu, Wenyu; Crawley, Matchew Lantz: Sparks,
Richard Bruce; Pruitt, James Russell; Takvorian, Amy
PATENT ASSIGNEE(S): Nincy Corporation, USA
DOCUMENT TYPE: LANGUAGE: PIXXD2

DOCUMENT TYPE: English
English
English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

OTHER SOURCE(S):

	PATENT NO.										APPL							
	WO 2005035551								WO 2	004-		20041007						
	WO	2005	0355	51		A3		20060908										
		W:	AE.	AG.	AL.	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
									DK,									
									IL,									
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		nu.							MZ,									
		F. W.							TJ,									
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	US	2005	2727	78		Al		2005	1208		US Z	004-	20041007					
	US	7141	596			B2		2006	1128									
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											US 2	003-	5293	72P		P 2	0031	211
											US 2	004-	£005	0 C D		P 2	0040	911

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention provides 1-oxo and 1,1-dioxoisothiazolones (shown

I-TV: also isothiazolidinone analogs of I-TV with R16 and R17 in place of R15 and R2 as a substituent at the 5 position of the isothiazolidinone ring; variables defined below: e.g. V) and related compds. that can modulate (no data) the activity of a target protein, such as a phosphatase, that selectively binds phosphorylated peptides or proteins. The present compds. can be useful (no data) in treating diseases or

CASREACT 142:411350; MARPAT 142:411350

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)phenyl-1-(5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl)piphenyl-4-sulfonamide 850315-63-55-55-550315-60-1P, 4-Bromo-H-([13)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-(5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-44-5P, N-[(18)-2-[4-(1,1-Dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 850315-69-9P, N-[(18)-2-(4-[1,1-Dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-2-(trifluoromethoxyl)benzenesulfonamide trifluoroacetate 850315-63-6P N, N-[(18)-2-[3-chloro4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)biphenyl-4-sulfonamide trifluoroacetate 850315-65-0P 850315-69-4P

4-Bromo-N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-73-0P(,N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 850327-65-0P 850327-67-2P, N-[(15)-1-(5-Chloro-1H-

benzimidazol-2-yl)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-69-4P, N-{(1S)-1-{5-Chloro-1H-benzimidazol-2-yl)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-71-8P,

N-[(18)-1-(5-chloro-1H-benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)phenyl|ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 80327-73-0P, N-[(18)-1-(5-chloro-1H-

benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-75-2P, N-[(15)-1-(3-chloro-1H-benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-77-4P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-79-6P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-83-2P, N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide

2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenylethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-85-49, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3, 4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-69, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-89-89, 3-chloro-N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenyl)-sthyl)-benzenesulfonamide trifluoroacetate 850327-91-2P, N-[(1S)-1-(5-chloro-1H-

benzimidazo1-2-y1)-2-[3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3-fluorobenzenesulfonamide trifluoroacetate

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) disorders, including, for example, diabetes and obesity, that are connected directly or indirectly to the activity of the target protein. Methods of prepn. are claimed and hundreds of example prepns. are included. For example, V was prepd. in 12 steps [50, 62, 100, 59, not detd., 100, 100, 99, not detd., not detd., 43, and 25 % yield) starting from N-tert-butyl-3-[2-(tert-butylcarbamoyl) ethyldisulfanyl)propionamide. For I-IV: a dashed line indicates an optional bond; Scl is a lst mol. scaffold or is absent; Sc2 is a 2nd mol. scaffold or is absent, wherein

least one of Sc1 and Sc2 is present; or Sc1 and Sc2 together with X1 and X2 or X4 and X5 form a 5-, 6-, or 7-membered fused carbocyclic ring or a 5-, 6-, or 7-membered fused heterocarbocyclic ring; X1 is C or N when Sc1 is present; X1 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc1 is absent; X2 is C or N when Sc2 is present; X2 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2 wherein the ring formed by X1, X2, X3, D1, D2, and D3 is an arom. ring; X4 is C or N when Sc1 is present; X4 is O, S, CR3, N, NR4,

CS, SO, or SO2 when Sc1 is absent; X5 is C or N when Sc2 is present; X5

O, S, CR3, N, NR4, CO, CS, SO, or SO2 when Sc2 is absent; X6 is C or N. Each E1 and E2 = O, S, CR3, N, NR4, CO, CS, SO, or SO2, wherein the rin formed by X4, X5, X6, E1, and E2 is an arom: ring; R2 is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl, OR26, SR28, NO2, CN, SOR29, SOR29, COR30, CORO31, NR32R33, a 5- or 6-membered heterocarbocyclyl group, or tetrazolyl. R15 is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl,

tetrazoly1. R15 is H, halo, cl-c4 alky1, C3-C6 cycloalky1, haloalky1,

C1-C4 alkoxy, C1-C4 haloalky1), SO(C3-C6 cycloalky1), SONRZ, SO3H, SO(C1-C4 alky1), SO(C1-C4 haloalky1), SO(C3-C6 cycloalky1), SONRZ, SO3H, SO2(C1-C4 alky1), SO(C1-C4 haloalky1), SO(C3-C6 cycloalky1), SONRZ, SO3H, SO2(C1-C4 alky1), CO(C1-C4 alky1), NC(C1-C4 alky1), CO(C1-C4 alky1), CO(C1-C4

phenylpropionyl]amino]-N-pentyl-3-[4-(1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]propionamide 850315-24-[P, N-[(1S)-2-[4-(1,1-Dioxido-4-

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 850327-93-4P, N-{(15)-1-(1H-Benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thladiazo1didin-2-y1)phenyl)ethyl]-3-chlorobenzenesulfonamide trifluoroacetate 850327-95-6P, N-{(15)-1-(1H-Benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-thladiazolidin-2-y1)phenyl}ethyl]-3-fluorobenzenesulfonamide trifluoroacetase RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; prepn. of 1-oxo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated

peptides and proteins)
850315-19-4 RCAPLUS
L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)-N-pentyl- (9CI) (CA INDEX

Absolute stereochemistry.

850315-22-9 HCAPLUS BB0315-22-9 nCAPD05 L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-24-1 HCAPLUS
[1,1'-Biphenyl]-4-sulfonamide, N-[(lS)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

RN 850315-36-5 HCAPLUS

Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl}-4(trifluoromethyl)-, mono(trifluoroacetate) [9CI] (CA INDEX NAME)

CM 1

CRN 850315-35-4 CMF C25 H19 F6 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide,
N-[(15)-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl|-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-43-4 CMF C26 H18 F9 N5 O5 S2

Absolute stereochemistry.

RN 850315-48-9 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-2-{4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phnyl]-1-{5-trifluoromethyl}-1H-benzinidazol-2-y1}ethyl]-2(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-47-8 CMF C25 H19 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CMF C2 H F3 O2 (Continued)

650315-40-1 HCAPLUS
Benzenesulfonamide, 4-bromo-N-[{15}-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-39-8 CMF C25 H18 Br F6 N5 O6 S2

Absolute stereochemistry.

850315-44-5 HCAPLUS

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 2

76-05-1 C2 H F3 O2

850315-63-8 HCAPLUS . [1,1'-Biphenyl]-4-sulfonamide, N-[(15)-2-[3-chloro-4-[1,1-dioxido-4-oxo-

1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-, mono(trifluoromethate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-62-7 CMF C30 H23 C1 F3 N5 O5 S2

r—с-со2н

850315-65-0 HCAPLUS
Benzenesulfonamide, N-{(1\$)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-4-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-64-9 CMF C25 H18 C1 F6 N5 O5 52

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-73-0 HCAPLUS
Benzenesulfonamide, N-{(1S)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-y1)phenyl}-1-{5-(trifluoromethyl)-1H-benzimidazol-2-y1)ethyl}-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-72-9 CMF C26 H17 C1 F9 N5 O5 52

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO2H

RN 850315-69-4 HCAPLUS
CN Benzenesulfonamide,
4-bromo-N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-68-3 CMF C25 H17 Br C1 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 850327-65-0 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-64-9 CMF C23 H19 C12 N5 O5 S2

RN 850327-67-2 HCAPLUS
CN Benzenesulfonamide,
N-[(15]-1-{5-chloro-lH-benzimidazol-2-yl}-2-{3-chloro4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-2-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-66-1 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-69-4 HCAPLUS

(Continued) ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-73-0 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxy-, monottrifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-72-9 CMF C25 H23 C12 N5 O7 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-,
mono(trifluoroacetate) [9CI] (CA INDEX NAME)

CM 1

CRN 850327-68-3 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

СМ

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-71-8 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-70-7 CMF C29 H23 C12 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-75-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-y1)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-74-1 CMF C25 H23 C12 N5 O5 S2

2

со2н

850327-77-4 HCAPLUS

Benzenesulfonamide, N-[(1s)-1-(1H-benzimidazol-2-yl)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl|phenyl]ethyl}-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-76-3 CMF C23 H20 C1 N5 O5 S2

Absolute stereochemistry.

ANSWER 6 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenesulfonamide, N-{(18}-l-(18-benzimidazo1-2-y1)-2-{3-chloro-4-(1,1-dioxido4-4-oxo-1.2,5-thiadiazolidin-2-y1)penyl}ethyl}-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-80-9 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-83-2 HCAPLUS
Benzenesulfonamide, N-[(15)-1-(1H-benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3-phenoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-82-1 CMF C29 H24 C1 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-79-6 HCAPLUS
Benzensulfonamide, N-{\ls\-1-(lH-benzimidazol-2-yl\-2-\ls\-chloro-4-\ls\-1,l-dioxido-4-\chloro-4-\chloro-4-\ls\-1,l-dioxido-4-\chloro-4-

CM 1

CRN 850327-78-5 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-81-0 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850327-85-4 HCAPLUS
Benzenesulfonamide, N-{(15)-1-(1H-benzimidazo1-2-y1)-2-{3-chloro-4-{1,1-dioxido4-e-avo-1,2,5-chiadiazolidin-2-y1)phenyl]ethyl]-3,4-dimethoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-84-3 CMF C25 H24 C1 N5 O7 S2

CM 2

850327-87-6 HCAPLUS
Benzenesulfonamide, N-[(|15)-1-(|H-benzimidazo1-2-y1)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-y1)pheny1]ethy1]-3,5-dimethy1-,
monottrifluoroacetate) (9CI) (CA INDEX NAME)

CM _1

CRN 850327-86-5 CMF C25 H24 C1 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN ' 76-05-1 CMF C2 H F3 O2

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

 $850327-93-4 \quad HCAPLUS \\ Benzenesulfonamide, N-\{\{1S\}-1-\{1H-benzimidazo1-2-y1\}-2-\{3-chloro-4-\{1,1-dioxido-4-xo-1,2,5-chloridiazolidin-2-y1\}phenyl\}=3-chloro-, \\ mono(trifluoroacetate) \\ \{9CI) \quad (CA \ INDEX \ NAME) \\ \\$

CRN 850327-92-3 CMF C23 H19 C12 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 850327-88-7 CMF C23 H18 C13 N5 O5 S2

Absolute stereochemistry.

CM 2

RN 850327-91-2 HCAPLUS
CN Benzenesulfonamide,
N-{(1S)-1-{S-chloro-1H-benzimidazo1-2-y1}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chliadiazo1idin-2-y1}phenyl}ethyl}-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-90-1 CMF C23 H18 C12 F N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO2H

850327-95-6 HCAPLUS
Benzenesulfonamide, N-{(1s)-1-(1H-benzimidazo1-2-y1)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl}-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-94-5 CMF C23 H19 C1 F N5 OS S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 850315-20-7P, ((5)-2-[4-(5-Benzyl-1,1,4-

trioxo[1,2,5]thiadiazolidin-2-yl)phenyl}-1-(pentylcarbamoyl)ethyl]carbamic
acid tert-butyl ester 850315-21-8P, {(1S)-1-{(1S)-2-(4-(5Benzyl-1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl)-1(pentylcarbamoyl)ethyl]carbamoyl)-2-phenylethyl]carbamic acid tert-butyl

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) ester 850315-23-DP, (2S)-3-[4-(5-Benzyl-1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]-2-[([2S)-2-[(2-(4-methoxyphenyl)acetyl)amino]-3-phenylpropionyl]lamino]-M-pentylpropionamide RL: RCT (Reactant): SPN (Synthetic preparation): PRPP (Preparation): RACT (Reactant or reagent) (prepn. of 1-oxo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins)
850315-20-7 HCAPLUS
Carbamic acid, [(15)-1-[(4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)phenylmethyl)-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-21-8 HCAPLUS L-Phenylalaninamide, N-{(1,1-dimethylathoxy)carbonyl}-L-phenylalanyl-4-{1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-23-0 MCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN

ED Entered STN: 11 Apr 2005
ACCESSION NUMBER: 2005:308290 HCAPLUS
DOCUMENT NUMBER: 143:7658
AUTHOR(S): Expedient syntheses of sulfonylhydantoins and two six-membered analogs aix-membered analogs
AUTHOR(S): Campbell, Andrew D.: Birch, Alan M.
Research and Development, AstraZeneca, Cheshire, SK10
4TG, UK
SUNCE: SYNLES: ISSN: 0936-5214
Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 143:7658
GI

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(\$): GI

A range of α -smino esters can be turned into sulfonylhydantoins in a single, atom-economic step using sulfamide and DBU. E.g., reaction of BMHCH2CO2CH with sulfamide and DBU gave 65% sulfonylhydantoin I. This procedure obviates the need for a three- or four-step sequence utilized AB

traditional procedures. Two new six-membered analogs [5-aryl-1,2,6-thiadiazinan-3-one 1,1-dioxides and 5-aryl-1,2-thiazinan-3-one 1,1-dioxides), e.g. II and III, have also been prepared utilizing novel synthetic protocols.
612528-23-1P 612529-46-1P 612530-69-5P 852358-50-0P 852358-51-1P 852358-53-3P 852358-54-4P 652358-56-P 852358-57-7P RL: SPN (Synthetic preparation); PREP (Preparation) IT

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (prepn. of sulfonylhydantoins via reaction of amino acid esters with sulfamide and DBM) 612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{2-phenylethyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

сн₂ — сн₂ — Рһ

612529-46-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{2-bromophenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

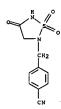
612530-69-5 HCAPLUS 1,2,5-Thiadizolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA HNDEX NAME)

852358-50-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2-chlorophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-51-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

852358-53-3 HCAPLUS Benzonitrile, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9CI) (CA INDEX NAME)



852358-54-4 HCAPLUS

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR 20

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

852358-56-6 HCAPLUS 032330-30-0 hoursus 1,2,5-Thiadiazolidin-3-one, 5-([1,1'-biphenyl]-3-ylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

852358-57-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-methyl-5-(phenylmethyl)-, 1,1-dioxide, (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 08 Mar 2005
ACCESSION NUMBER: 2005:202894 HCAPLUS
DOCUMENT NUMBER: 142:366767
TITLE: 142:366767
L2,5-7-thiadiszolidin-3-one 1,1-dioxide-based heterocyclic sulfides are potent inhibitors of human

AUTHOR(S):

AUTHOR(S):

AUTHOR(S):

Wong, Tzutshin; Groutas, Christopher S.; Mohan,
Swathir Lai, Zhong; Alliston, Kevin R.; Vu, Nga;
Schechter, Norman M.; Groutas, Wichita State University,
Wichita, KS, 67260, USA

SOURCE:

Archives of Biochemistry, Wichita State University,
Wichita, KS, 67260, USA

Auchives of Biochemistry and Biophysics (2005),
436(1), 1-7

CODEN: ABBIA4; ISSN: 0003-9861

PUBLISHER:

PUBLISHER:

DOCUMENT TYPE:

Journal

LANGUAGE:

AT the authors describe herein the design, synthesis, and in vitro biochem.
evaluation of a series of potent, time-dependent inhibitors of the mast
cell-derived series protesse tryptase. The inhibitors were readily
obtained by attaching various heterocyclic thiols, as well as a basic
primary specificity residue Pl, to the 1,2,5-thiadiszolidin-3-one
1,1-dioxide scaffold. The inhibitors were found to be devoid of any
inhibitory activity toward a neutral (elastase) or cysteine (papain)
protease, however they were also fairly efficient inhibitors of bovine
trypain. The differential inhibition observed with trypsin suggests that
enzyme selectivity can be optimized by exploiting differences in the 5'
substees of the two enzymes. The results described herein demonstrate

versatility of the heterocyclic scaffold in fashioning mechanism-based inhibitors of neutral, basic, and acidic (chymo)trypsin-like serine

IT

proteases. 849415-30-1P 849415-31-2P 849415-32-3P RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides are

potent inhibitors of human tryptase)
849415-30-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-2-[(2-benzoxazolylthio)methyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-31-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-[{{5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-32-3 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

849415-24-3P 849415-25-4P 849415-26-5P 849415-27-6P 849415-28-7P 849415-29-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

potent inhibitors of human tryptase)
849415-24-3 HCAPLUS
Carbamic acid, [4-{(35)-1,1-dioxido-4-oxo-2-{phenylmethyl}-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

849415-28-7 HCAPLUS
Carbamic acid, [4-[(3S)-1,1-dioxido-4-oxo-2-(phenylmethy1)-5-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-29-8 HCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-{phenylmethyl}-5-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

849415-25-4 HCAPLUS
Carbanic acid, (4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5[(phenylthio]methyl]-1,2,5-thiadiazolidin-3-yl]bucyl]-, phenylmethyl

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-26-5 HCAPLUS
Carbamic acid, [4-[(35)-5-(chloromethyl)-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester

(CA INDEX NAME)

Absolute stereochemistry.

RN 849415-27-6 HCAPLUS
CN Carbamic acid,
[4-[(35)-5-[(2-benzoxazolylthio)methyl]-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester
(9CI)

(CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 19 Aug 2004 ACCESSION NUMBER: 2004:677210 HCAPLUS

DOCUMENT NUMBER: 141:235669

AUTHOR (5):

141:235669
Potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin-3-one 1,1 dioxide-based
sulfonamide derivatives
Lai, Zhong; Gan, Xianqdong; Wei, Liuqing; Alliston,
Kevin R.; Yu, Hongyi; Li, Yue H.; Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Archives of Biochemistry and Biophysics (2004),
429(2), 191-197
CODEN: ABBIA4: ISSN: 0003-9861
Elsevier CORPORATE SOURCE:

SOURCE:

Archives of Biochemistry and Biophysics (2004),
429(2), 191-197
COODEN: ABBIA4: ISSN: 0003-9861
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:235669
AB The design, synthesis, and in vitro biochem. evaluation of a class of mechanism-based inhibitors of human leukocyte elastase (HLE) that incorporate in their structure a 1,2.5-thiadiazolidin-3-one 1,1-dioxide scaffold with appropriate recognition and reactivity elements appended to it is described. The synthesized compds. were found to be efficient, time-dependent inhibitors of HLE. The interaction of the inhibitors with HLE is postulated to lead to the formation of a highly reactive
N-sulfonyl innine (a Michael acceptor) that arises from an enzyme-induced sulfonamide fragmentation cascade. Subsequent reaction ultimately leads to the formation of a relatively stable acyl enzyme. The results cited herein demonstrate convincingly the superiority of the
1,2,5-thiadiazolidin-3-one
1,1 dioxide scaffold over other scaffolds (e.g., saccharin) in the design of inhibitors of (chymoltrypsin-like serine proteases.
17 49866-31-07 479866-31-07 479866-31-07 479866-31-07 479866-31-07 179866-3

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 212331-99-2P 749866-30-6P
RL: PRP (Properties): RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by 1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
RN 212331-99-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

749866-30-6 HCAPLUS Ethanethioic acid, S-[[(48)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester (9CI) (CA INDEX

Absolute stereochemistry.

220869-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by
,5-chiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
220869-64-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

749866-32-0 HCAPLUS
D-Phenylalanine, N-{[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl}-, methyl ester
(9C1) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-33-9 HCAPLUS
L-Phenylalanine, N-[[[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, phenylmethyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-34-0 HCAPLUS

'ASYGNE-34-U HARFLUS LE-Phenylalnine, N-[[{(48)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 30 Jul 2004 ACCESSION NUMBER: 2004:610081 HCAPLUS DOCUMENT NUMBER: 141:157120

141:157120
Preparation of sulfahydantoins as phosphate isosteres for use as phosphatase inhibitors in the treatment of cancer and autoimmune disorders
Saunders, Jeffrey O.; Miknis, Gregory F.; Blake, TITLE:

INVENTOR(S): James

PATENT ASSIGNEE(S): SOURCE: Vertex Pharmaceuticals Incorporated, USA

PCT Int. Appl., 62 pp. CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

		TENT																
	WO	2004	0626	64		A1				1	WO 2	003-		20031230				
		W:	AE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	ΒY,	BZ,	CA,	CH,	CN,
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			GM.	HR.	HU.	ID.	IL.	IN,	IS.	JP.	KE.	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
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								TJ,										
								HU.										
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	CA	2511	818			A1		2004	0729		CA 2	003-	2511	818		2	0031	230
	ΔII	2003	3004	47		Al		2004	0810		AU 2	003-	3004	47		2	0031	230
	116	2004	1671	87		A1		2004	0826	1	115 2	003-	7491	21		2	0031	230
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											wo 2	003-	11041	630	,	w 2	0031	230

MARPAT 141:157120

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
4-[1,1,4-Trioxo-[1,2,5]thiadiarolidin-2-yl)benzoic acid methyl ester
729600-47-9P 729600-48-0P 729600-49-1P
729600-50-4P 729600-51-5P 729600-52-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapputic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of sulfahydantoins as phosphate isosteres for use as protein

phosphatase inhibitors in treatment of cancer and autoimmune

disorders)
RN 612527-99-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

01

612530-69-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA

INDEX NAME)

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ' (Continued)

The invention relates to compds. having a sulfahydantoin or a reverse sulfahydantoin moiety (I) and (II) or pharmaceutically acceptable salts thereof [Q = each (un)substituted C1-8 aliphatic group, C6-10 aryl, heteroaryl having 5-10 ring atoms, heterocyclyl having 3-10 ring atoms; T = C1-6 alkylidene chain wherein one or two nonadjacent methylene units of T are optionally and independently replaced by O, NR, S, CO, CONR, NRCO, NRCONR, SO, SOZ, NRSOZ, SOZNR, or NRSOZNR; m = 0,1; X = CHZ, CO, CF2; R = H or (un)substituted C1-8 aliphatic group or two R groups bound to the

nitrogen are taken together with the nitrogen to form a 3-7 membered heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen,

neterocyclic ring having 0-2 heteroatoms in addition to the nitrogen, rein said heteroatoms are independently selected from N, O, or S), uses thereof, and related methods. These compds, are inhibitors of phosphatases, particularly inhibitors of protein tyrosine phosphatase SHP-2 and are used in the treatment of various phosphatase mediated diseases such as proliferative diseases, autoimmune disorders, angiogenic disorders, and cancer. The autoimmune disease is selected from glomerulonephritis, rheumatoid arthritis, systemic lupus erythematosus, scleroderma, chronic thyroiditis, Graves' disease, autoimmune gastritis, diabetes, autoimmune hemolytic anemia, autoimmune neutropenia, thrombocytopenia, atopic dermatitis, chronic active hepatitis, mysathenia gravis, multiple sclerosis, inflammatory bowel disease, ulcerative colitis, Crohn's disease, psoriasis, or graft vs. host disease. The proliferative disease is selected from acute myelogenous leukemia, mic myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple

proliferative disease is selected from acute myelogenous feureman, mic myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple myeloma, and HTLV-1-mediated tumorigenesis. The angiogenic disorder is selected from solid tumors, ocular neovasculization, and infantile haemangiomas. The cancer is selected from colon, breast, stomach, and ovarian cancer. Thus, N-alkylation of Me 4-aminobenzoate by Et bromacateate in the presence of EtN at 60° for 2.5 days gave 4-[[(Ethoxycarbonyl)methyl]amino]benzoic acid Me ester which underwent N-sulfamoylation by sulfamoyl chloride in the presence of EtN in CHZC12 at room temperature overnight to give 4-[N-[(Ethoxycarbonyl)methyl]-N-sulfamoylamino]benzoic acid Me ester (III). Cyclization of III by treatment with NaOMe/MeON at room temperature overnight gave 4-(1,1,4-trioxo-1,2,5-thiadiazolidin-2-yl)benzoic acid Me ester (IV). IV showed ICSO of 1.0-100 µM against protein tyrosine phosphatase SHP-2. 612527-99-8P 612530-69-5P 729600-44-6P,

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

729600-47-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-48-0 MCAPLUS
Benzoic acid, 3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
methyl ester (9C1) (CA INDEX NAME)

729600-49-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-phenyl-2-propenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-50-4 HCAPLUS
Benzamide, 4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9c1) (CA INDEX NAME)

NH- (CH2) 4-Ph

729600-51-5 HCAPLUS Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

ин- сн₂- Рh

729600-52-6 HCAPLUS Benzamide, N-butyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 23 Jul 2004
ACCESSION NUMBER: 2004:589375 HCAPLUS
DOCUMENT NUMBER: 141:140459
Freparation of sulfamides as anti-cancer agents
INVENTOR(5): Proparation of sulfamides as anti-cancer agents
Flynn, Daniel L.: Petrillo, Peter A.
Deciphera Pharmaceuticals, Inc., USA
PCT Int. Appl., 168 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

PATENT NO. KIND DATE APPLICATION NO. DATE W0 2004060305 A2 20040722 W0 2003-US41425 20031226
W1 2004060305 A3 20050210
W1 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MM, MZ, NO, NZ, OM, PR, PI, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TM, TM, AT, BE, BS, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2004171075 Al 20040909 US 2003-746548 20031224 US 2004176395 Al 20040909 US 2003-74654607 20031224 CA 2511840 Al 20040729 CA 2003-2511840 20031226 EP 1590344 A2 20051102 EP 2003-8014980 20031226 EP 1590344 A2 20051102 EP 2003-8014980 20031226 EP 2003-8014980 A2 20051102 EP 2003-8014980 A2 20051102 EP 2003-8014980 A2 20051102 EP 2003-8014980 A2 20051266 CP 2003-17863 A2 20051266 CP 2003-17863 A2 20051266 CP 2003-80140049 A2 20031226 CP 200519765 TP 20060831 AP 2005-508623 A2 20031226 CP 200508976 A2 20051976 US 2002-437403P P 20021231 US 2002-437415P P 20021231 US 2002-437487P P 20021231 US 2003-463804P P 20030418 US 2003-746545 A 20031224 US 2003-746607 A 20031224 W 20031226 WO 2003-US41425

OTHER SOURCE(S):

MARPAT 141:140459

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Sulfamides, such as I, were prepared for use as anticancer agents which

by modulating the activation states of abl or bcr-abl α -kinase proteins. Thus, 4-MO2CC6H4CH2NHSO2NHCOR [R = pyrrolidino], prepared from 4-Me02CC6H4CH2NH2 and pyrrolidine, was treated with the pyrimidinylaminoaniline fragment to give I, which showed 10% inhibition

non-phosphorylated abl kinase at 10µM.
726192-44-5P 726192-45-6P 726192-60-5P
726192-61-6P
RI: PAC (Pharmacological activity); SPN'(Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of sulfamides as anti-cancer agents), 726192-44-5 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-methyl]-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)

726192-45-6 HCAPLUS

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-N-[4-methyl-3-[(4-phenyl-2-pyrimidinyl)amino]phenyl]- (9CI) (CA INDEX NAME)

726192-60-5 HCAPLUS
Benzamide, 4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl)-N-[4-methyl-3-(2-pyrimidinylamino)phenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

726192-61-6 HCAPLUS
Urea, N-{4-{3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]-N'-{4-methyl-3-{2-pyrimidinylamino}phenyl}- (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612527-99-8P 612528-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagont)
(preparation of sulfamides as anti-cancer agents)
612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]-,
methy1 ester (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-00-4 HCAPLUS Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 18 Jun 2004 ACCESSION NUMBER: 2004:493693 HCAPLUS DOCUMENT NUMBER: 141:364348 Preparation 141:54348
Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as inhibitors of protein tyrosine phosphatase 18 Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorln Astrazeneca AB, Swed., Astrazeneca UK Limited PCT Int. Appl., 48 pp. CODEN: PIXXD2
Patent
English
1

INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

TENT	INFOR	MATI	ON:															
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w	0 2004	0506	46		A1 20040617					WO 2	003-	GB51	20		20031126			
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IORI	TY APE	LN.	INFO	.:						GB 2	002-	2781	3		A 2	0021	129	

WO 2003-GB5120

W 20031126

OTHER SOURCE(S):

MARPAT 141:54348

Title compds. I [wherein Rl = H, (halogeno)alkyl, (hydroxy)alkoxy, alkylamino, etc.; R2 = H, (halogeno)alkyl, halogeno, alkoxy; R3 = alkylamido or (un)substituted alkyl; R4 = H, alkyl, (hetero)aryl; R5 = H

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue Acetamide, N-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methoxyphenyl)methyl)- (9CI) (CA INDEX NAME) (Continued)

705256-61-7 HCAPLUS
Butanamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)- (9CI) (CA INDEX NAME)

705256-67-3 HCAPLUS

ייטיבט־פירס הערבייט Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-א-methyl- (9CI) (CA INDEX NAME)

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) or alkyl; and pharmaceutically acceptable salts thereof; were prepd. as inhibitors of protein tyrosine phosphatase 1B (PTB1B). For example, 5-[4-(actamidomethyl)-2-methoxyphenyl]-1, 2, 5-thiadiazolidin-3-one 1,1-dioxide [II] was given in multi-step synthesis starting from 3-methoxy-4-nitrobenzyl alc. II showed inhibition of human PTB1B with IC50 value of 44µM. Thus, I and their pharmaceutical compns. are useful as inhibitors of protein tyrosine phosphatase 1B for the treatment of diabetes mellitus. 705256-50-4 P05256-514-BP 705256-55-9P 705256-61-TP 705256-67-3P 705256-61-P 705256-68-2-2P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(preparation of 5-phenyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide
derivs. as
inhibitors of protein tyrosine phosphatase 1B)
RN 705256-50-4 KCAPLUS
CN Accetandie, N-[4-(1,1-dioxide-4-oxo-1,2,5-thiadiazolidin-2y1)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-54-8 HCAPLUS
Benzeneacetonitrile, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(9CI) (CA INDEX NAME)

705256-55-9 HCAPLUS

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 705256-72-0 HCAPLUS Benzenepentanamide, N-{(4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Ph- (CH2) 4-C-

705256-78-6 HCAPLUS Acetamide, N-[(14-(3)-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)methyli- (9CI) (CA INDEX NAME)

705256-82-2 HCAPLUS
Acetamide, N-[2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl)- (9CI) (CA INDEX NAME)

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) alkoxy, C1-6 alkoxy-C1-6 alkoxy, aryloxy, aryl-c1-6 alkoxy, aryloxy-C1-6 alkoxy, heteroaryl-c1-6 alkoxy, c1-6 alkoxy, c1-6 alkoxy-C1-6 a they are attached form a 5-7 membered carbocyclic or heterocyclic ring; and R4 are selected such that (i) R3 = hydrogen, C1-6 alkyl, C1-6 alkynyl, C1-6 alkythio or halo and R4 = aryl, biaryl, heteroaryl, C2-6 alkynyl, C3-7 cycloalkyl, arylcarbonyl, hereroarylarylaryl-c2-6 alkynyl, aryl-c2-6 alkynyl or heteroaryl-c2-6 alkenyl, or (ii) R4 = H, C1-6 alkyl, C1-6 alkyl, C1-6 alkyl, c1-6 alkyl, c1-6 alkyl, c2-6 alkynyl, aryl-c2-6 alkyl, aryl-c2-6 alkenyl, aryl-c2alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6 alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6
alkyl,
C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkyl, halo; R6 = H, C1-6 alkyl;
wherein any aryl, biaryl or heteroaryl group is optionally substituted]
are prepd. These compds. are useful as inhibitors of protein tyrosine
phosphatase PTP1B for the treatment of diabetes mellitus. Thus,
4-tolylboronic acid was coupled with 5-(4-bromophenyl)-1,2,5thiadiazolidin-3-one in the presence of
tetrakis(triphenylphosphine)pallad
ium(0) [Pd(PPh3)4] and cesium carbonate in a mixt. of DMF, DME, EtOH, and
H2O at 170° for 600 s to give 5-(4'-Methyl-1,1'-biphenyl-4-yl)1,2,5-thiadiazolidin-3-one 1,1-dioxide.
1,2,5-thiadiazolidin-3-one 1,1-dioxide.
1,2,5-thiadiazolidin-1-dioxide.
1,2,5-thiadiazolidin-1-dioxide.
1,3,5-thiadiazolidin-1-dioxide.
1,4,5-thiadiazolidin-1-dioxide.
1,4,5-thiadiazolidin-1-dioxide.
1,6,27-50-03-59 692165-17-67
RL: PAC (Pharbacological activity); RCT (Reactant); SPN (Synthetic
preparation); RACT (Reactant or reagent); USES (Uses)
(Preparation of phenylthiadiazolidinones as inhibitors of protein
tyrosine

vine
phosphatase lB (PTPIB) for treatment of diabetes mellitus)
692765-08-5 KCAPLUS
[1,1'-shipheny]]-4-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-y1)-4'-methoxy- (9CI) (CA INDEX NAME)

HCAPLUS [1,1'-Biphenyl]-3-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 21 May 2004 ACCESSION NUMBER: 2004:412929 HCAPLUS DOCUMENT NUMBER: 140:423678 TITLE: Preparation of 5-(substituted phenyl) thiadiazolidin-3ones as inhibitors of protein tyrosine phosphatase 18 Birch, Alan Martin; Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 89 pp. CODEN: PIXXD2 Patent INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: . DOCUMENT TYPE: English LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. DATE 20031103 PATENT NO. KIND DATE 2004041799

Al 20040521 W0 2003-GB4721 20031103
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MM, MM, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, ES, GS, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GM, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BC, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, WO 2004041799 AU 2003278392 PRIORITY APPLN. INFO.: Al 20040607 AU 2003-278392 GB 2002-25986 20031103 A 20021107

WO 2003-GB4721

W 20031103

OTHER SOURCE(S): MARPAT 140:423678

AB The title compds. (I) or pharmaceutically acceptable salts thereof [Rl = H, halo, Cl-6 alkyl, Cl-6 alkoxy, Cl-6 alkylthio, halo-Cl-6 alkyl, halo-Cl-6 alkoxy, halo-Cl-6 alkylthio, hydroxy-Cl-6 alkoxy, dihydroxy-Cl-6

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CO2H

692764-76-4P 692764-77-5P 692764-78-6P
692164-89-7P 692764-80-0P 692764-81-1P
692164-82-2P 692764-83-3P 692764-81-1P
692164-85-5P 692764-86-6P 692764-87-7P
692764-85-5P 692764-86-6P 692764-97-P
692764-91-3P 692764-98-9P 692764-97-5P
692764-91-3P 692764-98-0P 692764-97-1P
692765-00-7P 692765-01-8P 692764-98-P
692765-00-7P 692765-01-8P 692765-02-P
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692765-31-3P 692765-61-3P 69276

phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
692764-76-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{4'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide {9CI) (CA INDEX NAME)

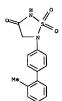
L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-77-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-nitro[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

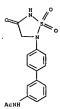
H N S

RN 692764-78-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-dichloro[1,1'-biphenyl]-4-yl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 692764-81-1 HCAPLUS
CN Acetamide, N-{4'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1){1,1'-biphenyl}-3-y1}- (9CI) (CA INDEX NAME)



RN 692764-82-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro[1,1'-biphenyl)-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-03-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (901) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-80-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692764-84-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(methylthio)[1,1'-biphenyl]-3-yl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-85-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-86-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2'-methyl{1,1'-biphenyl}-3-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-87-7 HCAPLUS
CN Acetamide, N-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl){1,1'-biphenyl}-3-yl}- (9CI) (CA INDEX NAME)

RN 692764-88-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[3-(2-benzofuranyl)phenyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 692764-89-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-93-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-4-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-94-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-95-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-fluoro-4-methoxy(1,1'-biphenyl)-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-90-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[3-(5-oxazolyl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-91-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-cyclohexylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-92-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-benzoylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Cont

RN 692764-96-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4,4'-dimethoxy[1,1'-bipheny1]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-97-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methowy-4'-phenoxy[1,1'-bipheny1]-3-y1)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-98-0 HCAPLUS
CN [1,1'-Biphenyl]-3-carbonitrile,
3'-(1,-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-99-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-nitro[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-00-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-01-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-hydroxy-4-methoxy{1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-05-2 HCAPLUS
CN Acetamide, N-{3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-4'methoxy{1,1'-biphenyl}-3-yl}- (9C1) (CA INDEX NAME)

RN 692765-06-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-methyl(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (921) (CA INDEX NAME)

RN 692765-07-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-acetyl-4-methoxy(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-02-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4,4'-trimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-{trifluoromethyl}[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-04-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(1,3-benzodioxol-5-yl)-2-methoxyphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Cont.

RN 692765-09-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1E)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-10-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-{2-naphthalenyl}phenyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-11-0 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-[4'-(hydroxymethyl)-4-methoxy[1,1'-biphenyl]-3-yl]-,1,1-dioxide (9CI) (CA INDEX NAME)

MeO CH2-OH

RN 692765-12-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-[methoxymethy1][1,1'-bipheny1]-3-y1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Heo CH2-OME

RN 692765-13-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

MeO NO CHAPPA

RN 692765-14-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-methoxy-4'-(phenylmethoxy) [1,1'-biphenyl]3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Meo CH2-OMe

RN 692765-19-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-methoxy-3'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

HeO N

RN 692765-20-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

H O N

RN 692765-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy{1,1'-biphenyl}-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

1.4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Meo O-CH₂-Ph

RN 692765-15-4 HCAPLUS CN 1,2,5-Thiadiazolidin-1-one, 5-[2-methoxy-5-[(12)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

M S Ph

RN 692765-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-[(1,1-dimethylethoxy)methyl]-4methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

Мео — СH2-ОВи-t

RN 692765-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-4'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Heo N

RN 692765-22-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-difluoro-4-methoxy[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

Meo Meo

RN 692765-23-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5'-fluoro-2',4-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

H ONE

RN 692765-24-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1':3',1''-terphenyl]-3-yl)-,
1,1-dloxide (901) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-25-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-27-8 RCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4'-(1,1-dimethylethyl)-4-methoxy{1,1'-biphenyl1-3-yl]-1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-3'-(trifluoromethyl){1,1'-biphenyl}-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[(1E)-2-(4-chlorophenyl)ethenyl]-2-methoxyphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-33-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-ethenyl-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-28-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy(1,1':4',1''-terphenyl)-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-29-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro-4'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-30-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1':4',1''-terphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 692765-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-furanyl)-2-methoxyphenyl]-,
1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-35-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-benzo[b]thien-2-yl-2-methoxyphenyl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-36-9 HCAPLUS CN 1,2,5-Thiddiazolidin-3-one, 5-[5-(2-benzofuranyl)-2-methoxyphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-37-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-38-1 HCAPLUS CN [1.1'-Biphenyl]-3-carboxamide, 3'-(1.1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-39-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[1H-pyrazol-4-yl)phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-40-5 HCAPLUS
CN Pyrrolidine, 1-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]carbonyl]- (SCI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-44-9 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, N-cyclohexyl-3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-amino-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 692765-46-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4'-(dimethylamino)-4-methoxy[1,1'-biphenyl]3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-41-6 HCAPLUS CN [1,1'-Biphenyl]-4-propanoic acid, 3'-(1,1-dioxido-4-oxo-1,2,5thiadiasolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-42-7 HCAPLUS
CN Carbamic acid, [(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA
INDEX NAMZ)

RN 692765-43-8 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Con

RN 692765-47-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(4-pyridinyl)phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-48-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-hydroxy-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-49-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[1H-indol-6-yl]-2-methoxyphenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-50-7 HCAPLUS
CN 1,2,5-Thladiazolidin-3-one, 5-(2-methoxy-5-(2-thienyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(phenylethynyl)phenyl)-,
1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-52-9 HCAPLUS
N 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(3-phenyl-1-propynyl)phenyl]-,
1,1-dtoxide (901) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-56-3 HCAPLUS

Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'
methoxy[1,1'-biphenyl]-3-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

RN 692765-57-4 HCAPLUS

Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methoxy)-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

RN 692765-58-5 HCAPLUS
CN Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-yl]methoxy]-6-hydroxy- (SCI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-53-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(5-ethynyl-2-methoxyphenyl)-, 1,1-dioxide (9C1) (CA INDEX NAME) ;

RN 692765-54-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methyl[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-55-2, HCAPLUS
CN Benzoic acid, 2-[2-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]ethoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 692765-59-6 HCAPLUS
CN Benzoic acid, 2-[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'-methoxy[1,1'-biphenyl]-4-yl]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-60-9 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]ethoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

RN 692765-61-0 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-62-1 RCAPLUS
Benzoic acid, 2-(3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy(1,1'-bipheny1)-3-y1)propoxy]-6-hydroxy- (9C1) (CA INDEX MAME)

692765-63-2 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-bipheny1)-3-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

692765-64-3 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]propoxy]-6-hydroxy- (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

692765-65-4 HCAPLUS
Bennoic acid, 2-[3-[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl)propoxy}-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-66-5 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]methoxy[-6-hydroxy- (9CI) (CA INDEX NAME)

RN 692765-67-6 HCAPLUS CN [1,1'-Biphenyl]-3-carboxamide, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy-N-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

NH-CH2-CH2-OPh

RN 692765-68-7 HCAPLUS
CN Benroic acid,
2-[2-[[[3]"-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester [9CI] (CA INDEX NAME)

692765-69-8 HCAPLUS

RN 692765-70-1 HCAPLUS
CN Benzoic acid,
C1[5-[[3]' (1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]carbony]amino]penty1]oxy]-6-hydroxy-, methyl
ester (9C1) (CA INDEX MAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-71-2 HCAPLUS
CN Benroic acid,
2-[[6-[[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]hexyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

RN 692765-72-3 HCAPLUS
CN Benzoic acid,
2-[2-[[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

RN 692765-73-4 HCAPLUS
CN Benroic acid,
2-[3-[[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl)-4-yl]carbonyl]amino]propoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-74-5 HCAPLUS
CN Benzoic acid,
2-[[5-[[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]carbony1]amino]penty1]oxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX NAME)

RN 692765-75-6 HCAPLUS
CN Benzoic acid,
2-[(6-[(3)*-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]carbonyl]amino]hexyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

692765-79-0P 692765-80-3P 692765-84-7P 692765-85-8P 692765-86-9P 692766-02-2P RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of phenylthiadiazolidinones as inhibitors of protein

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN methoxyphenyl]- (9CI) (CA INDEX NAME) (Continued)

692765-86-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-{4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

692766-02-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{5-iodo-2-methoxyphenyl}-, 1,1-dioxide

(CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phosphatase 18 (PP1B) for treatment of diabetes mellitus)
RN 692765-79-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-80-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-84-7 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 5-(5-bromo-2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-85-8 HCAPLUS Boronic acid, [3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 10 Oct 2003
ACCESSION NUMBER: 2003:796679 HCAPLUS
DOCUMENT NUMBER: 139:307766
TITLE: Preparation of substituted 1,1-dioxo-1,2,5thiazolidine-3-ones as protein tyrosine phosphatase 1b

and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis Coppola, Gary Mark, Davies, John William; Jewell, Charles Francis, Jr.; Li, Yu-chin: Wareing, James Richard: Spetbeck, Donald Mark; Stams, Travis Mathew; Topiol, Sidney Wolf; Vlattas, Isidoros Novartis A.-G., Switz.; Novartis Pharma G.m.b.H. PCT Int. Appl., 148 pp. CODEN: PIXXD2 Patent INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: Patent English 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

									APPLICATION NO.									
	WO	0 2003082841			A1 20031009			WO 2003-EP3466						20030402				
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MARPAT 139:307766

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Substituted thiazolidinetriones I (L1 = L2 = single bond, Q1 = single bond, H, (un)substituted alkyl, cycloalkyl, or aminocarbonyl, carboxy, RlOC(:O), RlOC(:O), RlOC(:O), RlOS(:O)q; Q2 = O, S, RRN, R, R2 = (un)substituted alkyl, alkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, aralkylthio, amino, halogen, nitro, carboxy, trifluoromethyl, etc.; Rl = (un)substituted alkyl, aryl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, aralkyl, RlO = (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, RlO = (un)substituted alkyl, aryl, heteroaryl, aryl aryloxycarbonyl, heteroaryloxycarbonyl, carbamoyl, or sulfonyl; X, Y = CH, N, O, S, Rl4N; Z = (un)substituted alkyl, alkoxyalkyl, alkylthioalkyl, alkylaminoalkyl; 2l, 22, 23 = CH, N, N(:O), CRl, CR2; Rl and R2 can form an (un)substituted 5 - or 6-membered aromatic or heteroarom. ring; Rl and Ll can form an (un)substituted 5-,

r 7-membered ring interrupted by nitrogen, oxygen or sulfur atoms) such as II are prepared as inhibitors of protein tyrosine phosphatase 1b and

protein tyrosine phosphatase for overcoming insulin resistance and modulating glucose levels in the treatment or prevention of metabolic diseases, such as diabetes, or atherosclerosis. II is prepared by ment

of Et bromoacetate with 1-naphthalenemethanamine, N-sulfamoylation with sulfamoyl chloride, and base-mediated cyclocondensation. No biol. data

provided.
612530-99-99 612530-90-2P 612530-92-4P 612530-93-5P 612530-94-6P 612530-95-7P 612531-03-68-8P 612530-98-0P 612531-03-99-1P 612531-00-7P 612531-01-8P 612531-02-9P 612531-03-0P 612531-03-9P 612531-13-2P 612531-13-3P 612531-13-3P 612531-13-4P 612531-13-65-9P 612531-13-14-7P 612531-31-65-9P 612531-31-61-0P 612531-31-65-9P 612531-61-0P 612531-65-5P 612531-66-5P ΙT

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-92-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[(2,4-dimethoxypheny])methyl]-5-[(4-methoxy7-quinolinyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-93-5 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, [4-(methylthio)phenyl)methyl ester (9CI)
(CA INDEX NAMEZ)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612531-67-6P 612531-68-7P 612531-69-8P
612531-70-1P 612531-75-6P 612531-76-P
612531-77-8P 612531-75-6P 612531-76-P
612531-77-6P 612531-78-9P 612531-79-0P
612531-69-3P 612534-94-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of thiezolidinetriones as protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosalerosis)
612530-69-9 RCAPLUS
Carbamic acid, [4-[(S-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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RN 612530-90-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-{(2,4-dimethoxyphenyl)methyl}-5-{(1-ethyl-2methyl-1H-benzimidazol-5-yl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

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612530-94-6 HCAPLUS

NN Benzoic acid,
4-([5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, [4-(methylsulfonyl)phenyl]methyl ester

(9CI) (CA INDEX NAME)

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RN 612530-95-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[bromomethyl]phenyl]methyl]-2-[[2,4-dimethoxyphenyl]methyl]-, 1,1-dioxide [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612530-98-0 HCAPLUS
CN Acetic acid, [[[4-[[5-{(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-chladiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-96-8 HCAPLUS
CN Acetic acid, [[[4-[[5-[[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo1,2,5-thiadiacolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Cor

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RN 612530-99-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-iodophenyl)mathyl]-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-00-7 HCAPLUS L-Phenylalanine, N-[{1,1-dimethylethoxy)carbonyl}-3-[[5-[{4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl], phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-01-8 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[5-[[4-

Absolute stereochemistry.

(Continued) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612531-05-2 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-10-9 HCAPLUS
CN Benzaldehyde,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-02-9 HCAPLUS
CN Carbamic acid,
[(1S)-1-{(3-[(5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612531-03-0 HCAPLUS Benzenepropanamide, α -amino-3-[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}-N-pentyl-, (α 5)-[9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 'ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

- 612531-13-2 HCAPLUS
1, 2, 5-Thiadiazolidin-3-one, 2-[(2, 4-dimethoxyphenyl)methyl]-5-[[4-[[4-[phenylmethyl]--]piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

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RN 612531-22-3 HCAPLUS
CN Carbamic acid, [[4-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-chiadiacolidin-2-yl]methyl]phenyl]methyl]-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)

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PAGE 1-A

RN 612531-23-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

t-Buo-C-NH-CH2-C-NH-CH2

CH2

N

CH2

MeO.

PAGE 2-A | Ome

RN 612531-30-3 HCAPLUS
CN Benzoic acid,
4-{[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-{aminomethyl)phenyl|methyl}-2-{(2,4-dimethoxyphenyl)methyl}-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

RN 612531-24-5 HCAPLUS
CN Carbamic acid
[2-[[4-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yl]methyl]phenyl]methyl]amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612531-31-4 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

612531-32-5 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, [4-((1,1-dimethylethoxy)carbonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-35-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-2-{(2,4-dimethoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-36-9 HCAPLUS
Benzoic acid, 3-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, methyl ester (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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612531-34-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-(2,4-dimitrophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-61-0 HCAPLUS
1H-1,4-Benzodiazepine-2,5-dione, 3-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-3-(phenylmethoxy)phenyl]methyl]-3,4-dihydro-(9CI)
(CA INDEX NAME)

RN 612531-63-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-64-3 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl)-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-65-4 HCAPLUS CN D-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-68-7 HCAPLUS
CN Benzenepropanamide, a-amino-4-[5-[(4-methoxyphenyl)methyl]-1,1dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612531-69-8 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-[5-[4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-66-5 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-4-{5-{(4-methoxyphenyl]methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 612531-67-6 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612531-70-1 HCAPLUS
CN L-Phenylalanine, 4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]-, phenylmethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-71-2 HCAPLUS
CN L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-{(4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, phenylmethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 612531-72-3 HCAPLUS
CN L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-{(4-methoxyphenyl)methyl}1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-73-4 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-[2-(1,1-dimethyxy)-2-oxoethyl]phenyl]ethyl]-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-77-8 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-{5-{{4-methoxyphenyl}nethyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-78-9 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[5-[4methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-75-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-76-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-2-((4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (

(Continued)

RN 612531-79-0 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yllphenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-80-3 HCAPLUS
Senzenepropanamide, α-amino-3-[5-{{4-methoxyphenyl}methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612534-94-8 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[5-[[4-.
methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

612527-93-2P 612530-46-8P 612530-49-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) , (invention compound; preparation of thiazolidinetriones as protein size.

e phosphatase 1b and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis) 612527-93-2 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-[(3-aminophenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN 612527-98-79 612528-00-4P 612528-01-5P 612528-02-6P 612528-00-4P 612528-01-5P 612528-02-6P 612528-01-1P 612528-01-6P 612528-11-7P 612528-12-8P 612528-13-9P 612528-13-9P 612528-11-7P 612528-12-8P 612528-13-9P 612528-11-7P 612528-12-8P 612528-13-9P 612528-13-9P 612528-13-9P 612528-13-9P 612528-23-9P 612528-23-9P 612528-23-P 612528-33-P 612528-33-P 612528-33-P 612528-34-P 612528-31-P 612528-33-P 612528-34-P 612528-34-P 612528-31-P 612528-33-P 612528-34-P 612528-34-P 612528-31-P 612528-31-P 612528-31-P 612528-42-P 612528-43-P 612528-43-P 612528-31-P 612528-51-P 612528-43-P 612528-51-P 612528-61-P 612528-71-P 6125

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-46-8 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
eater (9C1) (CA INDEX NAME)

612530-49-1 HCAPLUS
Benzeneacetic acid, 2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-,
methyl ester (9CI) (CA IMDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612530-04-8P 612530-05-9P 612530-06-0P
612530-08-2P 612530-09-1P 612530-10-6P
612530-11-7P 612530-12-8P 612530-13-9P
612530-16-2P 612530-17-3P 612530-18-4P
612530-29-P 612530-23-1P 612530-23-9P
612530-22-0P 612530-23-1P 612530-23-3P
612530-22-0P 612530-33-1P 612530-28-6P
612530-29-7P 612530-30-0P 612530-31-1P
612530-33-5P 612530-33-3P 612530-31-4P
612530-33-5P 612530-36-6P 612530-31-4P
612530-31-3P 612530-31-6P 612530-31-5P
612530-34-6P 612530-32-4P 612530-43-5P
612530-49-0P 612530-69-6P 612530-49-9P
612530-49-0P 612530-69-6P 612530-49-9P
612530-49-0P 612530-69-6P 612530-49-9P
612530-49-0P 612530-69-6P 612530-69-P 612530 (Uses)
(invention compd.; prepn. of thiazolidinetriones as protein tyrosine phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis)
612527-04-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(1-naphthalenylmethyl)-, 1,1-dioxide (9CI)

(CA INDEX NAME)

612527-85-2 HCAPLUS
Acetamide, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

612527-86-3 HCAPLUS
Carbamic acid, [{3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl]methyl}-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612527-87-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612527-88-5 HCAPLUS Acetamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-91-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[{3-iodophenyl}methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-92-1 MCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-94-3 HCAPLUS
Acetamide, N-{3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}- {9Cl} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-89-6 HCAPLUS
Carbamic acid, [[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612527-90-9 HCAPLUS
Benzenepropanamide, N-[[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl]phenyl]methyl}- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612527-96-5 HCAPLUS 1,2,3-Thiadiacolidin-3-one, 5-{(4-aminophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-97-6 HCAPLUS
Butanamide, N-[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl]- (9CI) (CA INDEX NAME)

RN 612527-98-7 HCAPLUS Urea, N-(3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-N'-612527-98-7 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN propyl- (9CI) (CA INDEX NAME) (Continued)

612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

612528-00-4 HCAPLUS
Benzoic acid, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(gCI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-07-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-08-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{4-amino-2-bromophenyl}methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-09-3 HCAPLUS
Acetamide, N-{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-01-5 HCAPLUS
Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]- .
(9CI) (CA INDEX NAME)

RN 612528-02-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methylphenyl)methyl]-, 1,1-dioxide
(9CI)

(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-10-6 HCAPLUS
Metheneulfonamide, N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]methyl]phenyl]- (9C1) (CA INDEX NAME)

612528-11-7 HCAPLUS
Methareaulfonaide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]nethyl]- (9Cf) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-12-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methylphenyl)methyl}-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612528-13-9 HCAPLUS

CN Benzeneacetic acid, α-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

N 612528-14-0 HCAPLUS
Benzeneacetamide, α-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-15-1 HCAPLUS
CN Benzeneacetamide, α-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-16-2 HCAPLUS
CN Benzeneacetamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]N-propyl-\alpha-[(trifluoroacety1)amino]- (9CI) (CA INDEX NAME)

RN 612528-17-3 KCAPLUS
CN Benzeneacetamide,
4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]a-((methylsulfonyl)amino]-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-18-4 HCAPLUS
CN Benzenepropanamide, α-(acetylamino)-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-19-5 HCAPLUS
CN Propanedioic acid, (acetylamino)[[4-[(1,1-dioxido-4-oxo-1,2,5-thididiazolidin-2-yl]methyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

RN 612528-20-8 HCAPLUS
CN Benzenepropanamide, α-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-21-9 HCAPLUS
CN Phenylalanine, N-acetyl-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-26-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{2-(2-chlorophenyl)ethyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-27-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(4-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-22-0 HCAPLUS CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-23-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-25-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3,4-dimethoxyphenyl)ethyl]-,
1,1-dioxide
(9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-28-6 HCAPLUS CN Acetamide, N-[4-[2-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)ethyl]phenyl]-2,2,2-trifluoro-(9CI) (CA INDEX NAME)

RN 612528-29-7 HCAPLUS
CN Butanamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]- (9CI) (CA INDEX NAME)

612528-32-2 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -(phenylmethyl)-,1,1-dioxide (9CI) (CA INDEX NAME)

R. 612528-33-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3-aminophenyl)ethyl]-, 1,1-dioxide (9CI)

(CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN 5-yl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

612528-37-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(4-methoxy-7-quinolinyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-38-8 HCAPLUS CN 1.2.5-Thiadiazolidin-3-one, 5-[[4-(2-methylpropoxy)-7-quinolinyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-39-9 HCAPLUS Glycine, N-[2-Cbutylamino)-2-oxo-1-phenylethyl]-N-[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-34-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{{4-(aminomethyl)-1-naphthalenyl}methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-35-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-36-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{[2-methyl-1-(3-methylbutyl)-1H-benzimidazol-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-40-2 HCAPLUS
Glycine, N-[2-(butylamino)-1-(4-ethylphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

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RN 612528-41-3 HCAPLUS
CN Glycine, N-[2-(butylamino)-2-oxo-1-(3-phenoxyphenyl)ethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzeyl]- (9CI) (CA INDEX NAME)

RN 612528-42-4 HCAPLUS
CN Glycine, N-[2-(butylamino)-1-(4-methoxyphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612528-44-6 KCAPLUS Clycine, N-[2-(butylamino)-1-(2-naphthalenyl)-2-oxoethyl]-N-[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612528-45-7 HCAPLUS CN Glycine, N-[2-(butylamino)-1-(4-chlorophenyl)-2-oxoethyl]-N-[4-[{1,1-doxido-4-oxo-1-2,5-chiadiazolidin-2-yl]methyl]benzoyl]- (9CI) (GA INDEX L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612528-43-5 HCAPLUS
CN Glycine, N-[1-(2-bromophenyl)-2-(butylamino)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued , NAME)

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N 612528-46-8 HCAPLUS
N Glycine, N-[2-(butylamino)-2-oxo-1-[3-(phenylmethoxy)phenyl]ethyl]-N-[4[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA
INDEX NAME)

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RN 612528-47-9 HCAPLUS
CN Glycine,
N-{(2E)-1-{(butylamino)carbonyl}-3-phenyl-2-propenyl}-N-{4-{(1,1-dioxido4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}benzoyl}- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 612528-48-0 HCAPLUS CN Glycine, N-[1-[[Utylamino]carbony1]-3-phenylpropy1]-N-[4-[(1,1-dioxido-4-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) PAGE 2-A

612528-50-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
(3-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

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612528-51-5 RCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl]-,
(4-butylphenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-49-1 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[4-(methylsulfonyl)phenyl]methyl ester {9Cl} (CA INDEX NAME)

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612528-52-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(hydroxymethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

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612528-53-7 RCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[2-(2-phenylethyl)menyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [4-(difluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)

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RN 612528-56-0 HCAPLUS
CN 2-Thiopheneacetic acid,
5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y[]methyl]benzoy]]oxy]methyl]-a,a-difluoro- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-54-8 RCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[1,1'-biphenyl]-2-ylmethyl ester (9CI) (CA INDEX NAME)

612528-55-9 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-57-1 HCAPLUS Acetic acid, [[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester [9CI) (CA INDEX NAME)

612528-58-2 HCAPLUS Acetic acid, [[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]hethyl]henyl]nethyl]thio]-, ethyl ester [9C1] (CA INDEX NAME)

RN 612528-59-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(3-methylbucyl)thio]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me2CH-CH2-CH2-5-CH2

RN 612529-60-6 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-ethylbutyl ester (9CI) (CA INDEX NAME)

RN 612528-61-7 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
cyclobutylmethyl ester (9CI) {CA INDEX NAME}

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-64-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2,4,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

RN 612528-65-1 MCAPLUS CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl)methyl]-, cyclohexylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-66-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-62-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
cyclopentylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-63-9 HCAPLUS CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-methylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-67-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclopentyl ester (9CI) (CA INDEX NAME)

RN 612528-68-4 HCAPLUS CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, 2-methylbutyl ester (9CI) (CA IMDEX NAME)

RN 612528-69-5 HCAPLUS
CN Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(methylthio)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-70-8 HCAPLUS
CN Benroic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-{(carboxymethyl)thio|ethyl ester (9CI) (CA INDEX NAME)

RN 612528-71-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(5-nitro-2-furanyl)methyl ester (9CI) (CA INDEX NAME)

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RN 612528-74-2 HCAPLUS
CM Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
[3-(methyl)ulfonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-72-0 HCAPLUS CN Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-pyridinylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-73-1 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[3-(hydroxymethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

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RN 612528-75-3 HCAPLUS
CN Benzeneacetic acid, 4-[4-[[4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]amino]butyl]- {9CI} (CA INDEX NAMÉ)

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612528-76-4 HCAPLUS
Benzeneacetic aid, 4-{3-{[(4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]methyl]benzoyl}amino|propyli- (9C1) (CA INDEX NAME)

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612528-77-5 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
[5-{(dimethylamino)methyl}-2-furanyl}methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-78-6 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612528-79-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(1H-indol-5-ylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-80-0 HCAPLUS
1,2,5-Thladiazolidin-3-one, 5-[(3,4,5-trimethoxyphenyl)methyl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

612528-82-2 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 5-[(4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-83-3 RCAPLUS Bernender (1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-plnmethyll- (9C1) (CA INDEX NAME)

612528-84-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-benzoylphenyl)methyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-85-5 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(2-naphthalenylmethyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612528-86-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(4-methyl-1-oxopentyl)phenyl]methyl]-,
1,-dioxide (SCI) (CA INDEX NAME)

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RN 612528-89-9 HCAPLUS CN 2(1H)-Quinolinone, 6-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

612528-97-9 HCAPLUS
Acetamide, 2-amino-N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]pheny1]methy1]- (9CI) (CA INDEX NAME)

612528-98-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-carboxyphenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-87-7 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[[3-(2-fluorophenoxy)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-88-8 HCAPLUS
Benzoic acid, 3-[2-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]ethoxy]- (9CI) (CA INDEX NAME)

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L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612528-99-1 HCAPLUS
1,2,5-Thiadiscolidin-3-one, 5-[(3-phenoxyphenyl)methyl]-, 1,1-dioxide
(SCI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-00-7 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-3-nitro- [9CI] (CA INDEX NAME)

612529-01-8 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[[4-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-02-9 HCAPLUS
Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-05-2 HCAPLUS
Benzoic acid, 5-amino-2-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1}- (9CI) (CA INDEX NAME)

RN 612529-06-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-methoxy-5-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-03-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-hydroxyphenyl)methyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

612529-04-1 HCAPLUS
Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-5-nitro- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-07-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-08-5 HCAPLUS
1,2,5-Thiadiacolidin-3-one, S-[(3-methyl-2-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-09-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-methylphenyl)methyl}-, 1,1-dioxide

(CA INDEX NAME)

612529-10-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-phenylpropyl)-, 1,1-dioxide (9CI) (CA

RN 612529-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-butoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

H N CH2

RN 612529-12-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

H N S CH2

- RN 612529-13-2 HCAPLUS
 CN Benzoic acid, 3-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]- (9CI) (CA INDEX NAME)
- L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

H O CH2

RN 612529-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methyl-3-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

CH2

RN 612529-17-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(5-methyl-2-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

02N CH2

RN 612529-18-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-aminophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

H₂N CO₂H

RN 612529-14-3 HCAPLUS
CN Benzenebutanoic acid,
5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

N N HO₂C-(CH₂)3

RN 612529-15-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methyl-3-nitrophenyl)methyl]-,
1,1-dioxide 90C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

H_N CH₂

RN 612529-19-8 HCAPLUS
CN 1H-Tsoindole-1,3(2H)-dione,
2-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

O CH2 - N NH

RN 612529-20-1 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-{[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

CH2 CH2 NH

RN 612529-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[1,4-phenylenebis(methylene)]bis-,
1,1,1'-tetraoxide (9CI) (CA INDEX NAME)

RN 612529-22-3 HCAPLUS
CN Acetic acid, [{2-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl]phenyl]amino]oxo- (9CI) (CA INDEX NAME)

RN 612529-23-4 HCAPLUS 1,2,5-Thiadiszolidin-3-one, 5-[(3-hydroxyphenyl]methyl]-, 1,1-dioxide (9c1) (CA INDEX NAME)

RN 612529-24-5 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

RN 612529-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-fluoromethy])phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, S-[[3-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-28-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-amino-5-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-29-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(3-amino-4-methylphenyl)methyl}-,
1,1-dioxide (921) (CA INDEX NAME)

RN 612529-30-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-3-methylphenyl)methyl)-,
1,1-dioxide (951) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612529-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-2-methylphenyl)methyl)-,
1,1-dioxide (921) (CA INDEX NAME)

RN 612529-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-amino-5-methylphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-33-6 HCAPLUS
CN Acetamide, N-[{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]-2,2,2-trifluoro-(9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612529-37-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-hydroxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-41-6 HCAPLUS
CN Benzoic acid, 2-amino-5-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-42-7 HCAPLUS
CN Benzoic acid,
2-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-43-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(phenylmethyl)phenyl]methyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-38-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, S-[(3,5-dimethylphenyl)methyl]-, 1,1-dioxide (961) (CA INDEX NAME)

RN 612529-39-2 HCAPLUS
CN L-Phenylalanine, N-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl}methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-40-5 HCAPLUS
CN L-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612529-44-9 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one, 5-[[2.4-bis(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-45-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2,4,6-trifluorophenyl)methyl]-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 612529-46-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-bromophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-47-2 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5,5'-[[1,1'-biphenyl]-2,2'-diylbis(methylene)]bis-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

612529-48-3 KCAPLUS
1,2,5-Thiadiacolidin-3-one, 5-[[4-[[ethylamino]methyl]phenyl]methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

612529-49-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Ph-CH2-CH2-NH-CH2

612529-52-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-{(diethylamino)methyl}phenyl]methyl]-,
1,-dioxide (9CI) (CA INDEX NAME)

612529-53-0 HCAPLUS
Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl|-, phenylmethyl ester (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CN Benzoic acid, 2-(acetylamino)-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]- (9CI) (CA INDEX NAME) (Continued)

612529-50-7 HCAPLUS Benzoic acid, 2-amino-4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}-, ethyl ester (9CI) (CA INDEX NAME)

RN 612529-51-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(2-phenylethyl)amino]methyl]phenyl]met hyl]-, 1,1-dioxide (9CI). (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-54-1 HCAPLUS
Benzamide, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 612529-56-3 HCAPLUS
CN Benzamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[2-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

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RN 612529-57-4 HCAPLUS
CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(3-methylbutyl)- (9CI) (CA INDEX NAME)

RN 612529-58-5 HCAPLUS CN 1,2,5-thiadiazolidine-2-acetic acid, $4-oxo-\alpha-(phenylmethyl)-$, 1,1-dioxide, $(\alpha S)-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry

RN 612529-59-6 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-α-{phenylmethyl}-,
1,1-dioxide, (αR)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-63-2 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-64-3 HCAPLUS
CN Acetic acid, (4-[(l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenoxyl-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-60-9 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

RN 612529-61-0 HCAPLUS CN Acetic acid, [4-(1),1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yllmethyl]phenoxyl- (9C1) (CA INDEX NAME)

RN 612529-62-1 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-65-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(carboxymethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)

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612529-67-6 HCAPLUS
Benzoic acid, 4-(2-([(4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y))methyl]phenyl]methyl]amino|ethyl]- (9CI) (CA INDEX NAME)

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ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-73-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-3nitro-, methyl ester (9CI) (CA INDEX NAME)

612529-74-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSMER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue 612529-68-7 HCAPLUS CN Acetic acid, [4+[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl|phenoxy|-, 2-methylpropyl ester (9CI) (CA INDEX NAME) (Continued)

612529-69-8 HCAPLUS
Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenoxy]-, phenylmethyl ester (9CI) (CA INDEX NAME)

612529-70-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-75-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-76-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[{4-ethoxyphenyl}methyl]-, 1,1-dioxide
(9CI) ,

(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-77-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-78-9 HCAPLUS
CN Benzeneacetic acid, 4-{{{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1}-benzoy1}oxy}methy1}- {SCI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-80-3 MCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(phenylamino)ethyl ester (9CI) (CA INDEX NAME)

RN 612529-81-4 HCAPLUS CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, 2-{3-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-79-0 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-phenylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-82-5 HCAPLUS

Senzoic acid, 4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl
ester (9CI) (CA INDEX NAME)

RN 612529-83-6 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-84-7 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-methoxy-2,2-dimethyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

RN 612529-85-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2,2,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-90-5 HCAPLUS
CN Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
(3-methyl-4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

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N 612529-91-6 HCAPLUS N Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-86-9 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
3-(dimethylamino)-2,2-dimethylpropyl ester {9CI} (CA INDEX NAME)

RN 612529-87-0 HCAPLUS

Senzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,

[(3aR,4s,5R,6aS)-5-(benzoyloxy)hexahydro-2-oxo-2H-cyclopenta[b]furan-4yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (3-chloro-4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

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RN 612529-93-8 HCAPLUS CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 6-thoxy-6-oxohoxyl ester (9C1) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-94-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(3-chlorophenyl)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-[3-(trifluoromethyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

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RN 612529-97-2 HCAPLUS D-Phenylalanine, N-[[4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-98-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(phenylmethyl)amino]methyl]phenyl]meth

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-95-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-(3-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)

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612529-96-1 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-99-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

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612530-01-5 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
[4-{methoxycarbonyl}phenyl]methyl ester (9CI) (CA INDEX NAME)

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ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612530-03-7 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-, 2-phenoxypropyl ester (9CI) (CA INDEX NAME)

612530-04-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612530-02-6 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-cyclohexyl-2-methylpropyl ester {9CI} (CA INDEX NAME)

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L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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612530-05-9 HCAPLUS
Benzoic acid, 4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[3-(trifluoromethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

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612530-06-0 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-(4-carboxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

612530-08-2 HCAPLUS
Benzoic acid, 3-[[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-10-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[(2,2-dimethylpropyl)amino]methyl]pheny
1]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me3C-CH2-NH-CH2

612530-11-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
l-naphthalenylmethyl ester (9CI) (CA INDEX NAMÉ)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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612530-12-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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DACE 2-8

N 612530-13-9 KCAPLUS

Benzeneaccic acid, 4-[2-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]amino|ethyl]- (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-

(Continued)

,

NO;

RN 612530-17-3 KCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-[(carboxymethyl)amino]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-18-4 HCAPLUS

14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

RN 612530-19-5 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
(1,1'-biphenyl]-4-ylmethyl ester (9C1) (CA INDEX NAME)

CH₂

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RN 612530-20-8 HCAPLUS

- L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN [Continued]
 CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 [4-(acetylamino)phenyl]methyl ester (9CI) (CA INDEX NAME)
 - H N S O CH2
 - PAGE 2-A

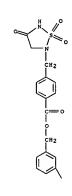
PAGE 1-A

- RN 612530-21-9 HCAPLUS
 CN Benzoic acid, 4-{[1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl}-,
 [2-(phenylmethyl)phenyl]methyl ester (9CT) (CA INDEX NAME)
- 14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (2-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)
 - N CH2 CH2 CH2
 - PAGE 2-A
- RN 612530-25-3 HCAPLUS

 Senzeneacetic acid, 3-[[[4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y])methyl]benzyl]oxy]methyl]- [9CI) (CA INDEX NAME)

- L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
- Ph-CH2
- RN 612530-22-0 HCAPLUS
 CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
 (2-methylphenyl)methyl ester (9CI) (CA INDEX NAME)
- CH2 CH2 Me
- RN 612530-23-1 HCAPLUS
 CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
- L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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- PAGE 2-A CH2-CO2H
- RN 612530-26-4 HCAPLUS
 CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
 (4-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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612530-27-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
[4-fluoro-2-(trifluoromethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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612530-29-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}methyl ester (9CI)
(CA INDEX NAME)

612530-30-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(5-methyl-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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RN 612530-28-6 HCAPLUS
CN Benzoic acid,
4-[(5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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612530-31-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylphenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

RN 612530-32-2 HCAPLUS

Senzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
3-((carboxymethyl)methylamino)-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-33-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-y1)methyl]-,
phenyl ester (9c1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-37-7 HCAPLUS
CN 1-Piperazineacetic acid, 4-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612530-38-8 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-naphthalenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-34-4 HCAPLUS

Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-[(2-methyl)propyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-35-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenylmethyl ester (9CI) (CA INDEX NAME)

RN 612530-36-6 HCAPLUS
CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N,N-bis(2-methylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-39-9 HCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]oxy]methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-40-2 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(aminocarbonyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-41-3 HCAPLUS
CN Piperazine, 1-[4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]bencyl]-4-[phenylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-42-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(1-oxo-3-phenylpropyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

612530-43-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-[[(phenylmethyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-48-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{4-{aminomethyl}phenyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

RN (CN ((9CI) 612530-50-4 HCAPLUS Benzeneacetic acid, 2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(CA INDEX NAME)

612530-51-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-dimethoxyphenyl)-, 1,1-dioxide, potassium salt (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-45-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{2,4-diaminophenyl}-, 1,1-dioxide (9CI) INDEX NAME)

612530-47-9 HCAPLUS Benzoic acid, 3-(1,1-dioxido-4-oxo¹1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-52-6P 612530-53-7P 612530-54-8P 612530-55-9P 612530-56-0P 612530-57-1P 612530-58-2P 612530-56-0P 612530-60-6P 612530-61-7P 612530-62-8P 612530-63-9P 612530-64-0P 612530-65-1P 612530-63-9P 612530-67-3P 612530-68-4P 612530-69-2P 612530-73-3P 612530-72-0P 612530-73-1P 612530-73-2P 612530-73-1P 612530-73-1P 612530-73-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-73-5P (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (es)

sine phosphatase 1b and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosolerosis) 612530-52-6 HCAPIUS Acetamide, 2-(4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-3-methylphenoxy]-N-(phenyimethyl)- (9CI) (CA INDEX NAME)

612530-53-7 HCAPLUS
1H-1,4-Benzodiezepine-2,5-dione, 3-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)-3-hydroxyphenyl]methyl]-3,4-dihydro- (9CI) (CA

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)

RN 612530-54-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-55-9 HCAPLUS

L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. .

RN 612530-56-0 RCAPLUS
CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry

RN 612530-60-6 HCAPLUS
CN L-Phenylalaninamide, N-benzoyl-O-(dicarboxymethyl)-L-tyrosyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-61-7 HCAPLUS
Senzenepropananide, α-{((1,1'-biphenyl)-4-ylsulfonyl)amino}-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 612530-57-1 RCAPLUS
CN L-Phenylalaninamids, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-58-2 HCAPLUS CN L-Phenylalaniamids, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-59-3 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-(carboxymethyl)phenyl]ethyl]-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612530-62-8 HCAPLUS
CN Benzenepropanamide, a=[([1,1'-biphenyl]-4-ylsulfonyl)amino]-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)-, (aS)-(SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-63-9 HCAPLUS
CN Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-a-[(phenylsulfonyl)amino]-, (aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-64-0 HCAPLUS

Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-(4-phenylbutyl)-a-{(phenylsulfonyl)amino}-, (aS)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 612530-65-1 HCAPLUS
CN Benzenepropanamide,
4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(3,3diphenylpropyl)-a-[(phenylsulfonyl)amino]-, (a5)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612530-66-2 HCAPLUS
CN L-Phenylalaninamide,
N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-{(4-aminophenyl)methyl}-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 612527-96-5 CMF C9 H11 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612530-72-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyl]-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612528-35-5 CMF C13 H16 N4 O3 S

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-67-3 HCAPLUS Benzenepropanamide, 3-bromo-4- $\{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]-N-(4-phenylbutyl)-<math>\alpha-\{(phenylsulfonyl)amino\}-, \{\alpha S\}-\{9CI\}$ (CA INDEX NAME)

Absolute stereochemistry.

612530-68-4 HCAPLUS L-Phenylalaninamide, tecyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-69-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-71-9 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM 2

CRN 76-05-1 CMF C2 H F3 O2

612530-73-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-([Z]-(3-oxo-2(3H)-benzofuranylidene)methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

612530-74-2 HCAPLUS Ethanedione, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}phenyl- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-75-3 HCAPLUS
9,10-Anthracenedione, 2-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}- (9CI) (CA INDEX NAME)

612530-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide, sodium salt (9CI) INDEX NAME)

● Na

612530-78-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{2,4-diaminophenyl}-, 1,1-dioxide, trifluoroacetate (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCE SAVALLABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

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L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

CM 1

CRN 612530-45-7 CMF C8 H10 N4 O3 S

CM 2

612534-93-7 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 31 Jul 2002

ACCESSION NUMBER: 2002:565367 HCAPLUS

DOCUMENT NUMBER: 137:323603

ITILE: AUTHOR(S): Efficient Solid-Phase Synthesis of Sulfahydantoins

Tremblay, Melanie: Voyer, Normand; Boujabi, Sihem; Dewynter, Georges F.

Centre de Recherche sur la Fonction, la Structure et l'Ingenierie des Proteines, Departement de Chimie, Faculte des Sciences et de Genie, Universite Laval, Quebec, QC, GIK 7P4, Can.

Journal of Combinatorial Chemistry (2002), 4(5), 429-435

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CODEN: JCHPF; ISSN: 1520-4766

American Chemical Society

Journal GI

CASREACT 137:232603

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB A novel solid-phase strategy allows the efficient preparation of traceless sulfahydantoins. A total of 28 derivs., with crude purity generally higher than 85%, were prepared by parallel synthesis. Through reductive alkylations, Mitsunobu reactions, and sulfamoylation reactions on oxime resim, the synthetic strategy affords sulfahydantoin derivs. selectively substituted at N2, e.g., I, N5, e.g., II, and N2, N5, e.g., III, positions, although yields of disubstituted compds. are lower. The mild reaction conditions involved, lead to sulfahydantoins without racemization.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
459831-33-5P 459831-34-6P 459831-35-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of N2,N5-disubstituted sulfahydantoins

reductive alkylation of resin-bound phenylalanine with substituted benzaldehydes and subsequent sulfamoylation, Mitsunobu reaction, resin-cleavage, and cyclization) 459831-33-5 HCAPIUS 1,2,5-Thiadiazolidin-3-one, 4-methylphenyl]methyl-4-[phenylmethyl)-2-(2-propenyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-34-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-butyl-5-[(4-methylphenyl)methyl)-4(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 459831-35-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methylphenyl)methyl]-4-(phenylmethyl)-2[3-phenylpropyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN 283587-14-4P 459831-30-2P 459831-31-3P 459831-32-4P (Continued) 459831-32-4P RL: SPN (39nthetic preparation); PREP (Preparation) (stereoselective preparation of N5-substituted sulfahydantoins via reductive

alkylation of resin-bound phenylalanine with substituted benzaldehydes
and subsequent sulfamoylation, resin-cleavage, and cycliration)

RN 283587-14-4 RCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methoxyphenyl)methyl)-4-(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-30-2 HCAPLUS Benzonitrile, 4-[([3S]-1,1-dioxido-4-oxo-3-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

459831-31-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-nitrophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCAPLUS 1,2,5-Thiadiazolidin-3-one, S-[(4-methylphenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSMER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 Oct 2001
ACCESSION NUMBER: 2001:735235 HCAPLUS
DOCUMENT NUMBER: 136:85785
TITLE: A one-step protocol for the N-chloromethylation of heterocyclic imides
AUTHOR(S): He, Shu; Yu, Hongyi; Fu, Qinghong; Kuang, Rongze;

Epp. Jeff B.: Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA

SOURCE: Synthetic Communications (2001), 31(20), 3055-3058

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): AB A convenient single step methodol. for the N-chloromethylation of heterocyclic imides using a mixture of formaldehyde sodium bisulfite adduct

and thionyl chloride is described. For example, the chloromethylation of 5-Butyl-3-propyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide gave. 387859-83-8 387859-86-1 RACT (Reactant or reagent) (preparation of 2-(chloromethyl-1,2,5-thiadiazolidin-3-one by chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 387859-83-8 HCAPIUS 1,2,5-thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 387859-86-1 HCAPLUS CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-{phenylmethyl}-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9P 387859-88-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 300553-65-9 HCAPLUS

JUUDD3-85-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{chloromethyl)-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

387859-88-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 5-(chloromethyl)-4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (SCI) (CA IN (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [{1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester (9CI) (CA INDEX NAME)

RN 220869-16-9 HCAPLUS CN Carbamic acid, [2-[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)- L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 13 Jun 2001 ACCESSION NUMBER: 2001:426029 HCAPLUS DOCUMENT NUMBER: 135:282665

DOCUMENT NUMBER: TITLE: 135:282665 Inhibition of serine proteases by functionalized sulfonamides coupled to the

1, 2, 5-thiadiazolidin-3-one

AUTHOR (5):

ne
1,1 dioxide scaffold
Groutas, W. C.; He, S.; Kuang, R.; Ruan, S.; Tu, J.;
Chan, H.-K.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (2001), 9(6),
1543-1548

CORPORATE SOURCE:

SOURCE:

1343-1348 CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd. PUBLISHER:

DOCUMENT TYPE: LANGUAGE: AB A challeng

NGG: Iffe: Souther VAGE: English A challenge associated with drug design is the development of selective inhibitors of proteases (serine or cysteine) that exhibit the same

inhibitors of proteases (Serine or cysesium, summary substrate specificity, i.e., show a preference for the same PI residue. While these proteases have similar active sites, nevertheless there are subtle differences in their S and S' subsites which can be exploited. We describe herein for the first time the use of functionalized sulfonamides as a design and diversity element which, when coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold yields potent, time-dependent inhibitors of the serine proteases human leukocyte elastase

1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold yields potent, time-dependent inhibitors of the serine proteases human leukocyte elastase

(HLE), proteinase 3 (PR 3) and cathepsin G (Cat G). Our preliminary findings suggest that (a) appending to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold recognition and diversity elements that interact with both the S and S' subsites of a target protease may result in optimal enzyme selectivity and potency and, (b) functionalized sulfonamides constitute a powerful design and diversity element with low intrinsic chemical reactivity and potentially wide applicability. Potent inhibitors of human leukocyte elastase, proteinase 3 and cathepsin G that interact with the S and S' subsites are realized by using functional sulfonamides coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold.

17 200869-05-67 200859-07-8P 200869-14-7P 200869-16-9P 365216-39-9P 365216-39-9P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified): PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea) (inhibition of serine proteases by functionalized sulfonamides coupled to 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)

NN 200869-05-6 HCAPLUS

CN Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl] (phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-yl]methyl1(methylsulfonyl)amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

365216-39-3 HCAPLUS

RN 365216-39-3 HCAPLU5
CN Benzamide,
N-[{4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5thiadia2olidin-2-yl}methyl}-N-{methylsulfonyl}- {9Cl} (CA INDEX NAME)
.

365216-41-7 HCAPLUS

Glycine,
[[[(4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](methylsulfonyl)amino)carbonyl}-, ethyl ester
(9CI) (CA INDEX NAME)

365216-42-8 HCAPLUS

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, butyl ester (9CI) (CA
INDEX
NAME)

RN 365216-43-9 HCAPLUS CN L-Phenylalanine, N-[[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-

(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carb onyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THIS THERE ARE 35 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 283587-15-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,4-dichlorophenyl)methyl}-4-(phenyl)e-thyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-16-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-18-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[{4(trifluoromethyl)phenyl]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS

L4 ANSWER 18 OF 33 RCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Apr 2001
ACCESSION NUMBER: 135:76831
TITLE: AUTHOR(\$): Albericio, Fernando; Bryman, Lois M.; Garcia, Javier; Michelotti, Enrique L.; Nicolas, Etnesto; Tice, Colin M.

CORPORATE SOURCE: Department of Organic Chemistry, University of Barcelona, Barcelona, 08028, Spain
OCUMEN: Journal of Combinatorial Chemistry (2001), 3(3), 290-300
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
JOURNAL AMERICAN CHEMICAL SOCIETY
AMERICAN CHEMICAL SOURCE(\$): CASREACT 135:76831
AB A five-step solid-phase synthesis of sulfahydantoins from q-amino acids and aldehydes was developed. The synthetic method allows the use of hindered amino acids, including Val, Phe, and Alb, and use of aromatic aldehydes substituted with electron-withdrawing and -donating groups. Some limitations were encountered with maino acids with reactive side chains. A small but diverse library of compds. was produced for biol. testing.

IT 201587-18-82 283587-15-5P 283587-16-6P 283587-18-82 346697-33-0P 346697-33-0P 346697-33-0P 346697-33-0P 346697-33-0P 346697-33-0P 346697-31-0P 34

L4 ANSMER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued N 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RM 283587-22-4 HCAPJUS
 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 283587-24-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[2(methylthio|sthyl]-, 1,1-dioxide, (45)- (5CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-35-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((3-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-36-7 HCAPLUS CN Acetamide, N-[4-[([35)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-Z-yl]methyl[phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-37-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(1-methylethyl)-5-(16-nitro-1,3-benzodioxol5-yl)methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-42-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[(4-(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (43)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-43-6 HCAPLUS
Acetamide, N-[4-[((3S)-1,1-dioxido-4-oxo-3-[(4-(phenylmethoxy)phenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-44-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4-[[4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, [45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 346697-38-9 HCAPLUS
CN 1,25-Thiadiacolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-39-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifuoromethyl)phenyl]methyl]4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-40-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-41-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[[4-(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-45-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-[(4-(phenylmethyp)phenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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Absolute stereochemistry.

RN 346697-47-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl)-4-[2-(methylthio)ethyl-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

346697-48-1 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-[2(methylchio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-49-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl]-4-[2-[methylthio)ethyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-50-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{[2-chloro-5-(trifluoromethyl)phenyl]methyl}4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
346697-55-0 HCAPLUS
1,2,5-Thicklatzolidin-3-one, 5-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4[((phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-56-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-57-2 HCAPLUS
1,2,5-Thiadiarolidine-3-acetic acid, 2-[(3-chlorophenyl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-58-3 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[[4-{acetylamino}phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-51-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2-chlorophenyl)methyl}-4[{(phenylmethyl)thio)methyl}-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

346697-53-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

346697-54-9 HCAPLUS Acetamide, N-[4-[(3R)-1,1-dioxido-4-oxo-3-[[(phenylmethyl)thio]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid,
2-{(4-chloro-3-nitrophenyl)methyl}-4oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-60-7 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2,4-dimethoxy-3-methylphenyl)methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-62-9 HCAPLUS CN 1,2,5-Thiadiszolidin-3-one, 5-[(4-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-63-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[2(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. .

RN 346697-64-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-65-2 HCAPLUS
CN Benzoic acid, 4-[([35)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yilmethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-73-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{{2-chloro-5-(trifluoromethyl)phenyl}methyl}4-{{4-(phenylmethoxy)phenyl]methyl}-, 1,1-dioxide, {4\$}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-74-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[(1(phenylmethyl)-1H-imidazol-4-yl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 346697-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-[{1-(phenylmethyl)-1H-imidazol-4-yl}methyl]- L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-69-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[(4(phenylmethoxyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-71-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[[4-(phenylmethoxy)phenyl]methyl]-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, [45)- (9CI) (CA INDEX NAMN)

Absolute stereochemistry.

RN 346697-72-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[(4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-76-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-y1)methy1)-4[[1-(phenylmethy1)-1H-imidazol-4-y1]methy1]-, 1,1-dioxide, (45)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 346697-77-6 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-methylphenyl)methyl]-4-oxo-,
methyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-79-8 HCAPLUS

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-[[4(trifluoromethyl)phenyl)methyl)-, methyl ester, 1,1-dioxide, (3S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry

RN 346697-80-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4-oxo-, methyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-81-2 HCAPLUS
CN Acetamide, N-[4-[[(35)-3-[2-(methylthio)ethyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl[phenyl]- [9CI] (CA INDEX NAME)

Absolute stereochemistry

RN 346697-82-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[2-(methylthio)ethyl]-5-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(4-chlorophenyl)methyl]-4-oxo-,
phenylmethyl este, 1,1-dioxide, (35)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-88-9 HCAPLUS
CN 1.2.5-Thiadiazolidine-3-acetic acid, 2-([6-nitro-1,3-benzodioxol-5-y1)methy1)-4-oxo-, phenylmethy1 ester, 1,1-dioxide, (38)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006'ACS on STN (Continued)

RN 346697-83-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chlorophenyl)methyl]-4[[(penylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

N 346697-84-5 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-{(2,4-dimethoxy-3-methylphenyl)methyl}-4-[[(phenylmethyl)thio|methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-85-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

14 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-89-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-90-3 HCAPLUS

N 1,2,5-Thiadiazolidin-3-one, 4-[(phenylmethoxy)methyl]-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-91-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[[phenylmethoxy]methyl]-5-[[3(trifluoromethyl]phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-92-5 HCÁPLUS
Benzoic acid, 4-[[{3S}-1,1-dioxido-4-oxo-3-[(phenylmethoxy)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-93-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4[(phenylmethoxy)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-97-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-{(4-nitrophenyl)methyl]-5-{{2-(crifluoromethyl)phenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) .

RN 346698-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-([2-(trifluoromethyl)phenyl]methyl], 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346698-04-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-phenyl-5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-05-3 HCAPLUS
Benzoic acid, 4-[(35)-1,1-dioxido-4-oxo-3-phenyl-1,2,5-thiadiazolidin-2yllmethyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{(4-nitrophenyl)methyl}-5-{(3-(trifluoromethyl)phenyl)methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

346697-99-2 HCAPLUS
Benzoic acid, 4-[[(35)-3-[(4-nitrophenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-00-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-[(4-nitrophenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346698-06-4 HCAPLUS 1.2,5-Thiadiszolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-phenyl-1,1-dioxide, (4S)- (9CI) {CA INDEX NAME}

Absolute stereochemistry.

346698-12-2 HCAPLUS
1,2,5-Thiadizcolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4-[(15)-1-methylpropyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

346698-14-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, S-{(4-methoxyphenyl)methyl]-4-{(15)-1-methylpropyl}-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 47 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Dec 2000
ACCESSION NUMBER: 2000:898004 HCAPLUS
DOCUMENT NUMBER: 134:307088

TITLE: 1,2,5-Thiadiazolidin-3-one 1,1 Dioxide: A Powerful Scaffold for Probing the S' Subsites of (Chymo)trypsin-Like Serine Proteases

AUTHOR(S): Grouts, William C.; Epp, Jeffrey B.; Kuang, Rongre; Ruan, Sumei; Chong, Lee S.; Venkataraman, Radhika; Tu,

Juan: He, Shu; Yu, Hongyi; Fu, Qinghong; Li, Yue He; Truong, Tien M.; Vu, Nga T. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Archives of Biochemistry and Biophysics (2001), 385(1), 162-169 CODEN: ABBITA4; ISSN: 0003-9861 Academic Press CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE:

LANGUAGE: English

The 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) embodies a motif that allows it to dock to the active site of (chymo)trypsin-like

eases
in a predictable and substrate-like fashion. Consequently, inhibitors
derived from this heterocyclic scaffold interact with both the S and S'
subsites of an enzyme. Exploitation of binding interactions with both

Sand S' subsites of a target enzyme may lead to compds. With greatly enhanced enzyme selectivity and inhibitory potency. This preliminary report describes the use of a series of compds. having the heterocyclic scaffold linked to various amino acids to probe the S' subsites of human leukocyte elastase (RLE), proteinase 3 (PR 3), and cathepsin G (Cat G). For comparative purposes, a series of compds. derived from a related scaffold, isothiazolidin-3-one 1,1 dioxide (II), was also generated. Several of the compds. were found to be highly potent and selective time-dependent inhibitors of HLE, PR 3, and Cat G. (c) 2001 Academic Press.
334975-68-7P 334975-69-8P 334975-69-8P 334975-68-39-393-98-1P
RL: BAC (Biological activity or effector, except adverse); BSU

RL: BAC (Biological activity or effector, except adverse); BSU

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PPP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold for probing S' subsites of human leukocyte elastase, proteinase 3 and cathepsin G) RN 314975-68-7 ROAPLUS (L.1-dioxide) (1,1-dioxide) (1,1-diox

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2

CRN 76-05-1 CMF C2 H F3 O2

CO2H

334975-81-4 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

334975-83-6 HCAPLUS L-Phenylalanine, ((43)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, monohydrochloride (9CI) (CA INDEX

334975-85-8 HCAPLUS

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

334975-69-8 HCAPLUS
D-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-, [(45)-4-{2-methylproyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-75-6 HCAPLUS
L-Phenylalanine, {(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, mono(trifluoroacetate) (9C1) (CA INDEX NAME)

CRN 334975-74-5 CMF C23 H29 N3 O5 S

Absolute stereochemistry

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) D-Phenylalanine, N-[(1,1-dimethylethoxy]carbonyl]-, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

344975-88-1 HCAPLUS
D-Phenylalanine, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME

CM 1

CRN 334975-87-0 CMF C26 H27 N3 O5 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT:

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl-2-oxazoly1)thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS 22003-23-7 m.crubs 1/2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-{((5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 19 Jul 2000 ACCESSION NUMBER: 2000:488727 HCAPLUS DOCUMENT NUMBER: 133:277919

DOCUMENT NUMBER: TITLE: Potent inhibition of serine proteases by heterocyclic sulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1

AUTHOR (5):

dioxide
He, S.; Kuang, R.; Venkataraman, R.; Tu, J.; Truong, T. M.; Chan, H. K.; Groutas, W. C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic 4 Medicinal Chemistry (2000), 8(7), 1713-1717

CORPORATE SOURCE:

SOURCE:

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:277919
AB The existence of subtle differences in the Sn' subsites of closely-related
(chymoltrypsin-like serine proteases, and the fact that the
1,2,5-thiediazolidin-1-one 1,1 dioxide scaffold docks to the active site of (chymoltrypsin-like enzymes in a substrate-like fashion, suggested that

that the introduction of recognition elements that can potentially interact with the Sn' subsites of these processes might provide an effective means for optimizing enzyme potency and selectivity. Accordingly, a series of heterocyclic sulfide derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) was synthesized and the inhibitory activity and selectivity of these compds. toward human leukocyte elastase (HLE), proteinase 3 (PR 3) and cathepsin G (Cat G) were then determined Compds. with Pl-misobutyl were found to be potent, time-dependent inhibitors of HLE and.

Pl-isobutyl were found to be potent, time-dependent inhibitors of RLE and, to a lesser extent PR 3, while those with Pl-benzyl inactivated Cat G rapidly and irreversibly. This study has demonstrated that 1,2,5-thiadiazolidin-3-one 1,1 dioxide-based heterocyclic sulfides are effective inhibitors of (chymoltrypsin-like serine proteases.

IT 220869-26-1P 220869-32-0P 220869-329-94P 220869-30-7P 220869-310-8-72 220869-30-7P 220869-310-8-72 220869-30-8-P 220869-310-8-P 22

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued) 220869-30-7 HCAPLUS 1,2,5-Thiadizoldin-3-one, 2-[(2-benzothiazolylthio|methyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-2-{[(5-phenyl-2-benzoxazolyl)thio]methyl}-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-39-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4,5-bis(phenylmethyl)-2-[([5-phenyl-1,3,4-oxadiazol-2-y])thio]methyl)-, 1,1-dioxide (9CT) (CA INDEX NAME)

220869-40-9 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 2-[([6-amino-2-benzoxazolyl)thio]methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (SCI) (CA INDEX NAME)

IT

300553-65-9 RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxide derivative; potent inhibition

serine protesses by heterocyclic sulfide derivs. of thiadisrolidinone dioxide)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 15 Jun 2000
ACCESSION NUMBER: 2000:335930 HCAPLUS
DOCUMENT NUMBER: 133:159438
TITLE: Utilization of the 1.2.5-thiad:

133:159638 Utilization of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold in the design of potent inhibitors

serine proteases: SAR studies using carboxylates Kuang, R.: Epp, J. B.: Ruan, S.; Chong, L. S.; Venkataraman, R.: Tu, J.: He, S.; Truong, T. M.: Groutas, W. C. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Bioorganic & Medicinal Chemistry (2000), 8(5), 1005-1016 AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd.

PUBLISHER:

CUMENT TYPE: LANGUAGE:

MENT TYPE: Journal
UNGE: English
A series of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one
1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds has been
synthesized and the inhibitory profile of these compds. toward human
leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3) was
then determined Most of the compds. were found to be potent,

then determined Most of the compos. Were sound to separative inhibitors of elastase, with some of the compos. exhibiting kinact/KI values as high as 4,928,300 ml s-1. The inhibitory potency of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform was found to be influenced by both the pKs and the inherent structure of the leaving group. Proper selection of the primary specificity group was found to lead to selective inhibition of HLE over Cat G, however, those compos. that inhibited HLE also inhibited PR 3, albeit less efficiently. The predictable mode of binding of these

is. Suggests that, among closely-related serine proteases, highly selective inhibitors of a particular serine protease can be fashioned by exploiting subtle differences in their S' subsites. 247179-63-19 267921-30-69 287921-33-9P 287921-73-79 267921-33-84 2 287921-35-9P 287921-42-0P 267921-45-3P 287921-46-4P 287921-52-2P 287921-54-4P 287921-55-7P 287921-91-9P 287921-91-9P 287921-52-4P 287921-54-BSU

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) ddy); PREP (Preparation) (synthesis of thiadiazolidinone dioxides and isothiazolidinone

dioxides

as serine protease inhibitors)
247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{acetyloxy}methyl]-4,5-bis(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

REFERENCE COUNT: THIS

THERE ARE 27 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-30-6 HCAPLUS CN Propanoic acid, 2,2-dimethyl-, [4-ethyl-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-33-9 HCAPLUS
Benzeneacetic acid, 4-[[(35)-5-[{2,2-dimethyl-1-oxopropoxy)methyl}-1,1-dioxido-4-oxo-3-propyl-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA

Absolute stereochemistry.

RN 287921-37-3 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[(43)-4-(2-methylpropyl)-1,1-dloxido-3-oxo5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

287921-38-4 HCAPLUS
Benzeneacetic acid, 4-[{(35}-5-[{2,2-dimethyl-1-oxopropoxy)methyl]-3-{2-methylpropyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-39-5 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 2-{(acetyloxy)methyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

287921-42-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(benzoyloxy)methyl]-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenepropanoic acid, {(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX

Absolute stereochemistry

287921-54-4 HCAPLUS
Benzeneacetic acid, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 287921-65-7 HCAPLUS
CN Benzoic acid, 2,6-dichloro-,
[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-91-9 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 2-[(acetyloxy)methyl]-4,5-bis(phenylmethyl)-,1,1-dioxide (9CI) (CA INDEX NAME)

1.4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-45-3 HCAPLUS

Senzoic acid, 2,6-dichloro-,
[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5[phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-46-4 HCAPLUS
Benzeneacetic acid, 4-{{\{35\}-5-{\{(2,6-dichlorobenzoyl)oxy]methyl}-3-{2-methylpropyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

287921-52-2 HCAPLUS

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 212331-98-1P 212331-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Reactant or reagent)
(Synthesis of thiadiazolidinone dioxides and isothiazolidinone dioxides

as serine protesse inhibitors)
RN 212331-98-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2((phenylthio)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{chloromethyl}-4-{2-methylpropyl}-5-{phenylmethyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THERE ARE 44 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 May 2000
ACCESSION NUMBER: 2000:324184 HCAPLUS
DOCUMENT NUMBER: 133:105000
TITLE: Solid-phase synthesis of sulfahydantoins
Albericio, Fernando; Garcia, Javier; Michelotti,
Enrique L.; Nicolas, Ernesto; Tice, Colin M.
Department of Organic Chemistry, University of
Barcelona, Barcelona, 08028, Spain
SOURCE: Tetrahedron Letters (2000), 41(17), 3161-3163
CODEN: TELEAY, 15SN: 0040-4039

PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): ASSEACT 133:105000
AB A S-atep solid-phase synthesis of 2-unsubstituted 1,2,5-thiadiazolidin-3one 1,1-dioxides, sulfahydantoins, from Na-Faoc amino acids and
aromatic aldehydes is described. The key step is the base-mediated
cyclitive
cleavage of a resin bound Na-aminosulfonyl Na-benzyl amino

Absolute stereochemistry.

283587-15-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS
1.2,5-Thiadiarolidin-3-one, 5-{(4-methoxyphenyl)methyl]-4,4-dimethyl-,1,1-dioxide (9CI) (CA IMDEX NAME)

283587-24-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl)-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 283587-16-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 4-(1-methylethyl)-5-([4(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (48)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dihydro-1,4-benzodioxin-6-y1)methyl]-4-(1-methylethyl)-, 1,1-dioxide, {45}- (9CI) {CA INDEX NAME}

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

29

REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 27 Aug 1999
ACCESSION NUMBER: 1999:536604 HCAPLUS
131:295863
131:295863
131:295863
AUTHOR(S): 131:295863
Bioorganic 4 Medicinal Chemistry, Michita State University, Wichita, KS, 67260, USA
Bioorganic 4 Medicinal Chemistry Letters (1999), 9(15), 2199-2204

PUBLISHER: 150:295864
Bioorganic 4 Medicinal Chemistry Letters (1999), 9(15), 2199-2204
CODEN: BMCLES: ISSN: 0960-894X
Elsevier Science Ltd.
DOCUMENT TYPE: 150:295864
AB A series of compds. that utilize the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold was synthesized and shown to be highly effective inhibitors of recombinant human skin chymase.

IT 170918-99-7 247178-61-2 247179-63-1
247179-64-2 247179-65-6 247179-63-7
247179-70-0 247179-71-2 247179-71-2 247179-71-55-5 247179-77-2 247179-74-4 247179-75-5 247179-77-2 247179-74-4 247179-75-5 247179-76-6
RL: BBC (Biological activity or effector, except adverse); BSU (Biological study) RI: BAC [Bloidgical activity of effector, except access, but
study, unclassified); PRP (Properties); BIOL (Biological study)
(human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold)
RN 170918-99-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
CN Acetic acid, hydroxy-,
[{4S}-1,1-dioxido-3-xov-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl}methyl ester (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

RN 247179-66-4 HCAPLUS
CN Propanoic acid, 2-hydroxy-,
[(48)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-67-5 HCAPLUS Benzeneacetic acid, α -hydroxy-, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{acetyloxy}methyl]-4,5-bis(phenylmethyl)-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-64-2 HCAPLUS
Propanedioic acid, mono([(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl) ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 247179-65-3 HCAPLUS

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

247179-68-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(methylsulfonyl)methyl}-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-69-7 HCAPLUS Acetic acid, [[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

247179-70-0 HCAPLUS
Propanoic acid, 3-[[[{45}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

247179-71-1 RCAPLUS
Benzoic acid, 2-[[([45]-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-72-2 HCAPLUS
Benzoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl}- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: THIS

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-74-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-{(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

247179-75-5 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 2-[[(6-amino-2-benzoxazolyl)thio]methyl)-4,5-bis(phenylmethyl)-, 1,1-dioxide, (48)- (9C) (CA INDEX NAME)

Absolute stereochemistry.

247179-76-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-{[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide, (45)- (9CI) {CA INDEX NAME}

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 25 Aug 1999 ACCESSION NUMBER: 1999:529816 HCAPLUS DOCUMENT NUMBER: 131:296959

A General Inhibitor Scaffold for Serine Proteases TITLE:

with

AUTHOR(S):

A General Inhibitor Scaffold for Serine Proteases

(Chymoltrypsin-Like Fold: Solution-Phase
Construction and Evaluation of the First Series of
Libraries of Mechanism-Based Inhibitors
Kuang, Rongre: Epp, Jeffrey B.; Ruan, Sumei; Yu,
Kongyi: Huang, Peng; He, Shu; Tu, Juan: Schechter,
Norman M.: Turbov, Jane: Froelich, Christopher J.;
Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Journal of the American Chemical Society (1999),
121(35), 8128-8129

CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

ISHER: American Chemical Society
MENT TYPE: Journal
UAGE: English
The authors demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1 dioxide
platform embodies a general motif that renders the platform capable of
binding to the active site of many serine proteases with a
(chymo)trypsin-like fold in a predictable fashion and is amenable to the
facile construction of libraries for lead identification and

facile constitution.

IT 170918-99-7P 170919-03-6P 189124-02-5P
247178-39-8P 247178-40-1P 247178-41-2P
RI: BAC (Biological activity or effector, except adverse); BSU

logical study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (inhibitor; general inhibitor scaffold for serine proteases with a (chymo)trypsin-like fold with solution-phase construction and

evaluation

uation

of first series of libraries of mechanism-based inhibitors)
170918-99-7 HCAPLUS
17,2,5-Thiddiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadizolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylminithyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry.

RN 189124-02-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-2-[(phenylaulfonyl)methyl]-4-propyl-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-39-8 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4-{4-aminobuty1}-5-{phenylmethy1}-2-{phenylmethy1}-1,1-dioxide, (45)-{9CI} (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 16 Mar 1999 ACCESSION NUMBER: 1999:172588 HCAPLUS DOCUMENT NUMBER: 130:209985

TITLE:

130:20985
Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as serine protease inhibitors Groutas, William C., Kuang, Rongze Wichita State University, USA PCT Int. Appl., 69 pp. CODEN: PIXXD2
Patent / English 1

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. DATE APPLICATION NO. DATE KIND WO 9909977 Al 19990304 WO 1998-US17406 19980821

W: AU, BR, CA, IS, JP, MX, NZ

RW: AT, BE, CH. CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

PT, SE

US 6420401 B1 20020716 US 1997-916693 19970822

AU 9990298 A 19990316 AU 1998-90298 19980821

EP 1011668 A1 20000628 EP 1998-942192 19980821

R: DE, GB

PRIORITY APPLN. INFO:: US 1997-916693 A 19970822 WO 1998-US17406 W 19980821

OTHER SOURCE(S):

MARPAT 130:209985

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247178-40-1 HCAPLUS

1,2,5-Thladiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-5-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[{(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) = G, H; m = 1-2; each R7 = amino acid side chain; each R8, R9 = alkyl, aryl, aralkyl, alkaryl, heterocyclyl; each R10-R15 = H, any group R8;

R16, R17 = heterocyclylalkyl; R18 = any group R8, NHR19; R19 = alkyl, aryl, aralkyl; with provisos], oligomers and combinatorial libraries contg. them, and methods of using them, are disclosed. Thus, title 1.

contg. them, and methods of using them, are disclosed. Thus, title dd.

II showed apparent second-order rate consts. Kinact/KI (M-ls-1) of 119,360, 27,400, and 60 for inhibition of human leukocyte elastase, proteinase 3, and cathepsin G, resp., by in vitro assays. 220868-4-6pp, combinatorial library derivs. 220868-85-Tpp, combinatorial library derivs. 220868-80-4DP, combinatorial library derivs. 220868-80-4DP, combinatorial library derivs. 220868-86-DP, combinatorial library derivs. 220868-81-1DP, combinatorial library derivs. 220868-87-DPP combinatorial library derivs. 220868-91-DP, combinatorial library derivs. 220868-91-DP, combinatorial library derivs. 220868-91-DP, combinatorial library derivs. 220868-91-DP, combinatorial library derivs. 220869-05-6P 220869-07-P 220869-07-P 220869-10-PP 220869-10-PP 220869-10-PP 220869-10-PP 220869-10-PP 220869-10-PP 220869-10-PP 220869-10-PP 220869-10-PP 220869-31-OP 320869-31-OP 320869-3

220869-41-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

as serine protease inhibitors)
RN 220868-74-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(4-methoxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 220869-75-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(3-phenoxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220668-80-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(acetyloxy)methyl}-5-{(4-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

220868-81-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(3-phenoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220868-92-8 HCAPLU5
CN L-Phenylalanine,
4-chloro-N-[[[[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3oxo-1,2,5-thiadiarolidin-2-yl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-93-9 HCAPLUS
L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]thio[methyl]-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-86-0 HCAPLUS
Carbamic acid, [[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3-oxo-1,2,5-thiadiazollidin-2-yl]methyl](methylsulfonyl)-, methyl ester [9CI) (CA INDEX NAME)

220868-87-1 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazollidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220868-98-4 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-99-5 HCAPLUS
L-Phenylalanine, 4-chloro-N-[{{[1,1-dioxido-3-oxo-5-[{3-phenoxyphenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]-(SCI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

220869-06-7 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, phenylmethyl ester (9CI)(CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220869-16-9 HCAPLUS
CN Carbamic acid,
[2-{[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl}(methylsulfonyl)amino]-2-oxoethyl)-,
phenylmethyl ester (9CI) (CA INDEX NAME)

220869-20-5 HCAPLUS ... 1,2,5-Thiadiscolidin-3-one, 2,2'-methylenebis[4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1,1',1'-tetraoxide (9CI) ... (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester (9CI) (CA INDEX

NAME)

RN 220869-14-7 HCAPLUS
CN Carbamic acid,
[2-[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-chiadiazolidin-2-yl]methyl](methylsulfonyl)amino}-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-26-1 HCAPLUS
1,2,5-Thiadisrolidin-3-one, 2-{(2-benzoxazolylthio)methyl}-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (901) (CA INDEX NAME)

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl-2-oxazoly1)thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-{{(5-

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-30-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[2-methylpropyl]-5-[phenylmethyl]-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-40-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{(6-amino-2-benzoxazolyl)thio}methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-41-0 HCAPLUS 1.2.5-Thiadiarolidine-2-acetic acid, α -fluoro-3-oxo-4.5-bis[phenylmethyl]-, ethyl ester, 1,1-dioxide, (48)- (9CI) (CA INDEX

Absolute stereochemistry.

220869-64-7 220869-65-8 RL: RCT (Reactant), PACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide deriva. IT

serine protesse inhibitors)
22089-64-7 KORPUS
1,2,5-Thiodiszolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-2-{[(5-phenyl-2-benzoxazolyl)thio]methyl]-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[(phnylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-39-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[[{5-phenyl-1,3,4-oxadiazol-2-yl}thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-65-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

220869-61-4P 220869-62-5P 220869-63-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derivs.

serine protesse inhibitors)
220859-61-4 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5(phenylmethyl)-, 1,1-dimethylethyl ester, 1,1-dioxide, (45)- (9CI) (CA
INDEX NAME)

220869-62-5 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-63-6 HCAPLUS
1,2,5-Thiadiazolidine-2-acetamide, 4-(2-methylpropyl)-3-oxo-N-(2-phenylethyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 15 CITED REFERENCES AVAILABLE FOR 15

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 02 Oct 1998 ACCESSION NUMBER: 1998:622789 HCAPLUS

TITLE:

SOURCE:

DOCUMENT NUMBER: 129:289796

129:289796
Kinetics of the hydrolysis of cyclic N-substituted sulfamides: 4-amino-2-cyclohexyl- and 4-amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5-thiadiazole 11,1-dioxides
Rozas, M. F.; Svartman, E. L.; Mirifico, M. V.; Vasini, E. J.
Instituto de Investigaciones Fisicoquimicas Te6ricas AUTHOR (5):

CORPORATE SOURCE:

Aplicadas (INIFTA), Facultad de Ciencias Exactas, Departamento de Quimica, Universidad Nacional de La Plata, La Plata, 1900, Argent. Journal of Physical Organic Chemistry (1998), 11(7), 489-494

CODEN: JPOCEE; ISSN: 0894-3230 John Wiley & Sons Ltd. Journal

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The hydrolysis reactions of 4-amino-2-phenethyl- and
4-amino-2-cyclohexyl2,3-dihydro-3-oxo-1,2,5-thiadiazole 1,1-dioxide (Ia and Ib) were
investigated at 24-73 in buffered aqueous solns. The observed rate
consts. (kobs) are independent of pH in the range ca 1-4 pH, but increase
with increase in pH above ca 4. A linear log kobs vs pH profile with

unit

slope is observed from pH ca 4 up to the highest exptl. pH (ca 10). The
products are the corresponding new compds.: 2-amino-2-[(N-substitutedsulfamoyl)imino]acetic acid salts. The C=N bond of these compds.
hydrolyzes further, in a slow reaction, to the sulfamide and oxalic acid
derivs. The substrates decompose to the final products without
accumulation

accumulation
of the acetic acid derivs, under these exptl. conditions. A mechanism is
proposed. Rate consts. and activation parameters are given for the first
reaction step. Owing to steric effects, the reaction rate is higher for
the N-phenethyl-substituted derivative than for the
2-cyclohexyl-substituted
derivative
IT 214216-09-8, 4-Amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5thiadiazole 11,1-dioxide
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
RCT

(Reactant); PROC (Process); RACT (Reactant or reagent)
 (hydrolysis of cyclic N-substituted sulfamides)
214216-09-8 HCAPLUS
1,2,5-Thiadiazol-3-amine, 4,5-dihydro-5-(2-phenylethyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 05 Aug 1998
ACCESSION NUMBER: 1998:487562 HCAPLUS
129:216561
Potent and specific inhibition of human leukocyte elastase, cathepsin G and proteinase 3 by sulfone derivatives employing the 1,2,5-thiadizablidin-3-one 1,1-doxide scaffold Grouts, William C.: Kuang, Rongze; Ruan, Sumei; Epp, Jeffrey B.: Venkateraman, Radhika; Truong, Tien M. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (1998), 6(6),

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd.

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: GI Journal English

This paper describes the results of structure-activity relationship studies in a series of heterocyclic mechanism-based inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold (I: Rl = iso-Bu, benzyl, RZ = Bu, Me, benzyl, RZ (RZCOCMSA), etc.; L = SOZPh, SOZCGHKG1-4, etc.) and capable of interacting with the Sn and S'n subsites of a serine proteinase. Sulfone derivs. of I were found to be highly effective, time-dependent inhibitors of human leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3). The judicious selection of an Rl group (accommodated at the primary specificity site S1) that is based on the known substrate specificity of a target serine proteinase, was found to yield highly selective inhibitors. The presence of a benzyl group (RZ = benzyl) at the S2 subsite was found to lead to a pronounced enhancement

inhibitory potency. Furthermore, the effective use of computer graphics and modeling has led to the design of potent, water-soluble inhibitors.

results of these studies demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1-dioxide platform provides an effective means for appending

IT

gmition
elements in a well-defined vector relationship, and in fashioning
highly-selective and potent inhibitors of serine proteinases.
21231-98-1P 21231-99-2P 21232-00-8P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation); RACT
(Reactant or reagent)
(1,2,5-thiadiazolidin-3-one 1,1-dioxide inhibitors of human leukocyte
electace cathepsin G and proteinase 3)
21231-39-1 HCAPLUS
2 5-Thiadiazolidin-3-one 4-(2-methyl)ropyl)-5-(phenylmethyl)-2-

212331-99-1 HCAPDUS 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[(phenylthio)methyl]-, l,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

212332-00-8 KCAPLUS
Benzeneacetic acid, 3-[((35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylthio]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-79-8P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

proteinase 3) 212331-79-8 HCAPLUS

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.
Double bond geometry as shown.

.
170919-03-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-77-6 HCAPLUS
Benzoic acid, 4-[[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-78-7 MCAPLUS
Benzoic acid, 4-[([35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5([phenylsulfonyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Befizoic acid, 3-[([35]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 170918-99-7P 170919-01-4P 170919-03-6P
212331-77-6P 212331-78-7P 212331-80-1P
212331-81-2P 212331-82-3P 212331-83-4P
212331-83-5P 212331-97-0P
212331-97-5P 212331-97-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3)
RN 170918-99-7 HCAPUUS
CN 1,2,5-Thiadiazolidin-1-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

N 170919-01-4 HCAPLUS N 1,2,5-Thiadiazolidin-3-one, -(phenylmethyl)-5-[(2E)-3-phenyl-2-propenyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

212331-80-1 HCAPLUS
Benzoic acid, 3-[([3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

212331-81-2 HCAPLUS
Benzoic acid, 2-[((35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-82-3 HCAPLUS Benzoic acid, 2-[[(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN · (Continued) ((phenylaulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 212331-83-4 HCAPLUS
CN Benzenesctic acid, 4-[[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl)- (9CI) (CA

Absolute stereochemistry.

RN 212331-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[[(4-chlorophenyl)sulfonyl]methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-92-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenylpropyl)sulfonyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-94-7 HCAPLUS (1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-([[3-(trifluoromethyl)phenyl]sulfonyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-95-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(2-phenylethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4-chlorophenyl)methyl]sulfonyl]methyl]-4{2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-97-0 HCAPLUS
CN Benzeneacetic acid, 4-[[(3S)-1,1-dioxido-4-oxo-3-(phenylmethyl)-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

.

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 09 Apr 1998
ACCESSION NUMBER: 1998:200895 HCAPLUS
DOCUMENT NUMBER: 128:278642
Use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent inhibitors of serine proteinases Kuang, Rongze; Venkataraman, Radhika; Ruan, Sumei; Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998),

BIOORGANIC 4 Medicinal Chemistry Letters (1998),

539-544
CODEN: BNCLES; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The attachment of a phosphate leaving group to the
1,2,5-thiadiazolidin-3one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds was found
to yield highly potent, time-dependent inhibitors of human leukocyte
elastase (HLE).

17 205932-85-0P 205932-87-2P 205932-88-3P
205932-89-4P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPN (Synthetic propagative)

logical
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and
isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent
inhibitors of serine proteinases)
205932-65-0 HCAPLUS
Phosphoric acid, dimethyl (4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX

205932-87-2 HCAPLUS Phosphoric acid, dibutyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo (phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI)

L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 30 Aug 1997 ACCESSION NUMBER: 1997:555602 HCAPLUS DOCUMENT NUMBER: 127:257045

Competitive particle concentration fluorescence immunoassays for measuring antidiabetic drug levels

AUTHOR(5):

mouse plasma Bright, Stuart W.; Tinsley, Frank C.; Dominianni, Samuel J.; Schmiegel, Klaus K.; Fitch, Lora L.; Gold, Gerald

Geraco Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA Journal of Immunological Methods (1997), 207(1), CORPORATE SOURCE:

SOURCE: 23-31

CODEN: JIMMBG; ISSN: 0022-1759

PUBLISHER: DOCUMENT TYPE:

LANGUAGE:

CODER: GARMEN; 155N: VU22-1759

R: Elsewier
TYPE: Journal
: English
competitive particle concentration fluorescence immunoassays were

developed to measure blood levels of analogs of antidiabetic drugs being tested in diabetic mice. Ligands that contained the active pharmacophores were conjugated to PPD for immunization and to β-phycoerythrin for use as a tracer in the immunoassays. Approx. 90% of 262 compds. assayed were detectable at less than 120 nM in plasma which was well below the estimated therepeutic level of 1 μM for lowering blood glucose. These data were used to define the bioavailability of test compds. and assist in decisions

sions
of constructing active analogs. Of addnl. interest, we noted
crossreactivity of one monoclonal antibody for 3 different compound

ses that are all known to bind with varying affinities to peroxisome proliferator-activated receptors. 196079-43-3

1960/3-43-3 RL: ANT (Analyte); ANST (Analytical study) (competitive particle concentration fluorescence immunoassays for

(competitive particle concentration fluorescence immuniossays for suring antidiabetic drug levels in mouse plasma)

196079-43-3 HCAPUUS

1,2,5-Thiadiarolidin-3-one, 5-[4-[2-(2-phenyl-4-oxazolyl)ethoxy]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR 13

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

205932-88-3 HCAPLUS
Phosphoric acid, [4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5-thiadiazolidin-2-yl]methyl bis(phenylmethyl) ester (9CI) (CA INDE NAME)

205932-89-4 HCAPLUS
Phosphoric acid, [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl diphenyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 09 Apr 1997
ACCESSION NUMBER: 1997:226843 HCAPLUS
DOCUMENT NUMBER: 126:287581
Structure-Based Design of a General Class of Mechanism-Based Inhibitors of the Serine Proteinases Employing a Novel Amino Acid-Derived Heterocyclic Scaffold

AUTHOR(S): Ground Milliam C.; Kuang, Rongre; Venkataraman, Radhika; Epp, Jeffrey B.; Ruan, Sumei: Prakash, Om Departement of Chemistry, Wichita State University, Wichita State Univ

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

JAGE: English
We describe in this paper the structure-based design of a general class

heterocyclic mechanism-based inhibitors of the serine proteinases that embody in their structure a novel peptidomimetic scaffold (1,2,5-thiadiazolidin-3-one 1,1-dioxide). Sulfone derivs. of this class were time-dependent, potent, and highly efficient irreversible inhibitors of human leukocyte elastase, cathepsin G, and proteinase 3. The

partition ratios for a select number of inhibitors were found to range between $\boldsymbol{0}$

and 1. We furthermore demonstrate that these inhibitors exhibit remarkable ${\bf r}$

selectivity that is dictated by the nature of the P1 residue and is consistent with the known substrate specificity reported for these enzymes. Thus, inhibitors with small hydrophobic side chains were effective inhibitors of elastase, those with aromatic side chains of cathepsin G, and those with a basic side chain of bovine trypsin. Taken together, the findings cited herein reveal the emergence of a general class of stable mechanism-based inhibitors of the serine proteinases

can be readily synthesized using amino acid precursors. Biochem. and high-field NMR studies show that the interaction of this class of inhibitors with a serine proteinase results in the formation of a stable acyl complex(es) and the release of benzenesulfinate, formaldehyde, and a low mol. weight heterocycle. The data are consistent with initial

formation of a Michaelis-Menten complex, acylation of Ser195, and tandem loss of

or a michaelis-Menten complex, acylation of Ser195, and tandem loss of leaving group. The initial HLE-inhibitor complex reacts with water generating formaldehyde and a stable HLE-inhibitor complex. Whether the initial HLE-inhibitor complex also reacts with His57 to form a third complex is not known at this point. The desirable salient parameters associated with this class of inhibitors, including the expeditious generation of structurally diverse libraries of inhibitors based on I, suggest that this class of mechanism-based inhibitors is of general applicability and can be used in the development of inhibitors of human and viral serine proceinases of clin. relevance.
170918-99-7P 170919-03-6P 189124-00-3P 189124-02-9P 189124-02-9P 189124-03-9P RL: BAC (Biological activity or effector, except adverse); BSU logical study, unclassified); SPN (Synthetic preparation); BIOL (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and structure activity relations of mechanism-based inhibitors

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) of human leukocyte serine proteinases employing a novel amino acid-derived heterocyclic scaffold) 170918-99-7 KCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

170919-03-6 KCAPLUS
1,2,5-Thiadiacolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylmulfonyl)methyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-00-3 HCAPLUS
1,2,5-Thiadizzolidin-3-one, 4-ethyl-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

14 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylmethyl)-2-(phenylmulfonyl)methyl)-4propyl-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-04-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{1-methylethyl}-5-{phenylmethyl}-2-{{phenylsulfonyl}methyl}-, 1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

189124-06-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-butyl-5-(phenylmethyl)-2-

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 01 Dec 1995
ACCESSION NUMBER: 1995:954574 HCAPLUS
123:340140
Novel serine protease inhibitors: derivatives of isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide Groutas, william C.

INVENTOR(S): Groutas, william C.
PATENT ASSIGNEE(S): Wichita State University, USA
PCT Int. Appl., 93 pp.
CODEN: PIXXD2
PATENT INFORMATION:
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

							D			APPLICATION NO.						DATE			
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												1995-				1	0050	102	

OTHER SOURCE(S): MARPAT 123:340140

Various isothiszolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiszolidine 1,1-dioxide derivs., e.g. I $\{X=CR2, \{un\}$ substituted NH; RI = H, alkyl, $\{un\}$ substituted benzyl, indolylalkyl, etc.; Y= non-steroidal antiinflammatory residue, H, protected amino acid, acyloxy, etc.], and their use to reduce or inhibit the activity of serine proteases, are claimed. The compds, are useful as anti-inflammatory and anti-metastatic agents. For example, 4-benzylisothiazolidin-3-one 1,1-dioxide underwent

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
N-alkylation with ClCH2SPh and Et3N in MeCN, followed by S-oxidn. with
m-ClC6H6(O)OOH in CH2C12 (904), to give title compd. II. In an in vitro
assay, II had an apparent 2nd-order inactivation rate const. (kobs/[I]

M-1
s-sssy, if and an appetent zind-totel finativation rate const. (KODS)(1)
s-1) of 960 against cathepsin G. A variety of compds. were prepd. and/or tested against cathepsin G, human leukocyte elastase, and/or proteinase-3.
If 170919-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
(intermediate; preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-16-1 RCAPLUS
CN 12,25-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-(3-phenyl-2-propenyl)-2((phenylthio)methyl)-, 1,1-dioxide, (S-(E))- (SCI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

IT 170919-15-OP
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or respent); USES (Uses)
(preparation of isothizolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-15-O HCAPLUS
CN 1.2,5-Thiadiazolidin-1-one,
4,5-bis(phenylmethyl)-2-[(phenylthio)methyl]-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

170919-03-6 170919-21-8 170919-22-9 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(Uses)

(Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-03-6 HCAPLUS
CN 1,25-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-21-8 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 4-(2-methylpropy1)-5-(phenylmethy1)-2-[(phenylsulfonyl)methy1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 170919-22-9 HCAPLUS

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 153044-45-2P 170918-99-7P 170919-01-4P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isothiazolidinone and oxothladiazolidine dioxide derivs. as serine protease inhibitors)
RN 153044-45-2 KCAPLUS
CN 12,25-Thiediazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-(2E)-3-phenyl-2-propenyl)-2-(phenylsulfonyl)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:124451 HCAPLUS
DOCUMENT NUMBER: 120:124451 SUbstituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides:
a new class of potential mechanism-based inhibitors

AUTHOR (S):

CORPORATE SOURCE:

human leukocyte elastase and cathepsin G
Groutas, William C.; Kuang, Rongze; Venkataraman,
Radhika
Dep. Chem., Wichita State Univ., Wichita, KS, 67260,
USA
Biochemical and Biophysical Research Communications
(1994), 198(1), 341-9
CODEN: BBRCA9; ISSN: 0006-291X
Journal
English

DOCUMENT TYPE: LANGUAGE: GI

A series of substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides (I, R = benzyl; RI = H, Me, benzyl, CH2CO2-tert-Bu or CH2CO2-benzyl) was prepd, and their in vitro inhibitory activity toward human leukocyte elastase

cathepsin G was investigated. These compds inactivated the 2 enzymes efficiently and in a time-dependent fashion.

IT 153044-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and human leukocyte elastase and cathepsin G
inhibition by)
RN 153044-45-2 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Jan 1991 ACCESSION NUMBER: 1991:23940 HCAPLUS

1991:23940 HCAPLUS

DOCUMENT NUMBER:

TITLE:

114:23940
Intra- and intermolecular α-sulfamidoalkylation reactions
Lee, Chai Ho; Kohn, Harold
Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA

AUTHOR(S): CORPORATE SOURCE:

USA Journal of Organic Chemistry (1990), 55(25), 6098-104 CODEN: JOCEAH; ISSN: 0022-3263 Journal

DOCUMENT TYPE:

SOURCE:

OTHER SOURCE(S):

English CASREACT 114:23940

5=0 PhCH2N 1

The utility of $\alpha\text{-sulfamidoalkylation}$ processes for the generation of sulfamidea has been examined Both intra- and intermol. a sulfamiodalkylation transformations were observed to proceed in moderate

good yields. The generality of these processes has been demonstrated using N.N'-di(aryl-substituted) sulfamides, and the utility of these reactions was examined for the preparation of cyclic sulfamides of novel structure. Thus, reaction of PhoRNNNSONINE with ELOZCCH(OEL)2 in the presence of CF3COZH gave 74% dithintetrazocinedicarboxylate tetraoxide I, whereas reaction of 3-MeOCGHACHNNSONINE with ELOZCCH(OEL)2 in CF3COZH followed by methylation gave benzothiadiarepinecarboxylate dioxide II. The crystal structures of I and II were determined 130670-00-7P

1306/0-00-79 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Reactant of reagent)
(preparation and cyclization of)
130670-00-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-hydroxy-5-(2-phenylethyl)-, 1,1-dioxide,
monosodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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         SEP 21
                 CA/CAplus fields enhanced with simultaneous left and right
                 truncation
         SEP 25
                 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS
     8
                 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS
     9
         SEP 25
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
         SEP 25
NEWS 10
                 CEABA-VTB classification code fields reloaded with new
NEWS 11
         SEP 28
                 classification scheme
                 LOGOFF HOLD duration extended to 120 minutes
NEWS 12
         OCT 19
NEWS 13
                 E-mail format enhanced
         OCT 19
                 Option to turn off MARPAT highlighting enhancements available
         OCT 23
NEWS 14
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 15
         OCT 23
                 multiple databases
                 The Derwent World Patents Index suite of databases on STN
         OCT 23
NEWS 16
                 has been enhanced and reloaded
                 CHEMLIST enhanced with new search and display field
NEWS 17
         OCT 30
                 JAPIO enhanced with IPC 8 features and functionality
         NOV 03
NEWS 18
                 CA/CAplus F-Term thesaurus enhanced
         NOV 10
NEWS 19
                 STN Express with Discover! free maintenance release Version
NEWS 20
         NOV 10
                 8.01c now available
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 21
         NOV 20
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NEWS 22
         NOV 20
                 to 50,000
NEWS 23
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                 CAS REGISTRY updated with new ambiguity codes
                 CAS REGISTRY chemical nomenclature enhanced
NEWS 24
         DEC 11
         DEC 14
NEWS 25
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                 GBFULL and FRFULL enhanced with IPC 8 features and
NEWS 26
         DEC 14
                 functionality
                 CA/CAplus pre-1967 chemical substance index entries enhanced
NEWS 27
         DEC 18
                 with preparation role
                 CA/CAplus patent kind codes updated
NEWS 28
         DEC 18
                 MARPAT to CA/CAplus accession number crossover limit increased
NEWS 29
         DEC 18
                 to 50,000
                 MEDLINE updated in preparation for 2007 reload
NEWS 30
         DEC 18
              NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
NEWS EXPRESS
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP)
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
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FULL ESTIMATED COST

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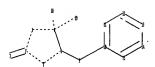
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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10510026RTR.str



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chain nodes :
7  9  18  19
ring nodes :
1  2  3  4  5  10  11  12  13  14  15
chain bonds :
2-7  4-18  4-19  5-9  9-10
ring bonds :
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exact/norm bonds :
1-2  1-5  2-3  2-7  3-4  4-5  4-18  4-19  5-9
exact bonds :
9-10
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15
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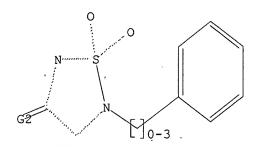
G1:H,CH3

G2:0,S

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me G2 O, S

Structure attributes must be viewed using STN Express query preparation.

=> s l1 SAMPLE SEARCH INITIATED 12:19:35 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 62 TO ITERATE

100.0% PROCESSED 62 ITERATIONS 50 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 768 TO 1712
PROJECTED ANSWERS: 576 TO 1424

L2 50 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 12:19:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1006 TO ITERATE

100.0% PROCESSED 1006 ITERATIONS 770 ANSWERS

SEARCH TIME: 00.00.01

L3 770 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'HCAPLUS' ENTERED AT 12:19:44 ON 21 DEC 2006
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=> s 13

L4 33 L3

=> d ed ibib abs hitstr 1-33

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 03 Aug 2006 ACCESSION NUMBER: 2006:765251 HCAPLUS DOCUMENT NUMBER: 145:211037 TITLE: Precision Pre 2006:765251 HCAPLUS
145:211037
Preparation of pyrazolyl aryl ureas as modulators of
the protein kinase activation state for treatment of
inflammation and hyperproliferative diseases
Flynn, Daniel L.; Petillo, Peter A.
Deciphera Pharmaceuticals, LLC, USA
PCT Int. Appl., 305pp.
CODEN: PIXXD2
Patent
English
2

INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT	INFOR	MATI	ON:															
P.F	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D	ATE		
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		CN,	co.	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
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		KZ.	LC.	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	ΜK,	MN,	MW,	MX,	
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		SG.	sĸ.	SL,	SM,	5Y,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	
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		CF.	CG.	CI.	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,	
							NA,											
					RU,													
PRIORIT	TY APP	LN.	INFO	. :						US 2	004-	6389	87P		P 2	0041	223	

MARPAT 145:211037

OTHER SOURCE(5):

Novel compds. and methods of using those compds. for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and diseases

characterized by hypervascularization are provided. In a preferred

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

PAGE 1-A

903567-40-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-3,4-dioxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl)-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(SCI) (CA INDEX NAME)

embodiment, the compds. of the invention modulate the activation state of p38 kinase protein, abl kinase protein, bcr-abl kinase protein, braf kinase protein, VEGFR kinase protein, cr PGFR kinase protein, braf compds. of the invention I have general formula (RI-(X)])m-A-NH-L-NH-D-(E)q-(Y)t-Q wherein RI = aryl, heteroaryl, and heterocylyl; X and Y = individually O, S, alkynyl, alkenyl, etc.; A = an arom., monocyloheterocyclic or bicycloheterocyclic ring; D = Ph or a 5-6-membered heterocyclic ring; E = Ph, pyridinyl, or pyrimidinyl; L = -C(O) - or -S(O)2-; j.m.qt = 0-1; and Q = a substituted ring or ring system. Over 500 compds. were prepd. For example, hydrogenation of 3-(3-aminophenyl) acrylic acid Me ester provided the propionate, which was subsequently converted to the hydrarine. Reaction of the hydrazine with 4.4-dimethyl-3-coxpentamenitrile afforded Me
3-[3-(3-test-butyl-5-amino-lH-pyrazole-1-yl)phenyl|propionate. which was coupled with 1-naphthyl isocyanate and reduced to provide urea II. In a competition assay with SKF 86002 as a fluorescent probe, II inhibited p38 MAP kinase with ICSO of

of

45 nM.
697369-58-3P 903567-40-8P
RL: DNA (Drug mechanism of action); PAC (Pharmacological activity); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrazolyl aryl ureas as modulators of
protein kinase activation state for treating inflammation and
proliferative disorders)
897369-58-3 HCAPLUS
Ulrea. τT

RN 897369-58-3 HCAPLUS
CN Urea,
N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-{(1,1-dioxido-3,4-dioxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-lH-pyrazol-5-yl)- (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-35-2P, 1-[5-tert-Bucyl-2-[3-[[(S)-3-methyl-1,1,4-trioxo-

[1,2,5] thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3- (naphthalen-1-yl)urea 872171-37-4P, 1-[5-text-Butyl-2-[3-]([R]-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3- (naphthalen-1-yl)urea 872171-57-6P, N-[3-text-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-2-naphthalenscarboxamide 872171-62-5P, 1-[5-text-Butyl-2-[3-

 $\begin{array}{l} \{(1,1,4-trioxo-\{1,2,5\}thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-yl]-2-$

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrazol-3-y1]-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]3-(4-methoxynaphthalen-1-yl)urea
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological atudy); PREP (Preparation); USES
(USes)

(p36 kinase inhibitor, preparation of pyrazolyl aryl ureas as modulators of

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-37-4 HCAPLUS
Urea, N-{3-1(,1-dimethylethyl)-1-{3-{([3R)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thidiazolidin-2-yl]methyl]phenyl}-1H-pyrazol-5-yl}-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-57-8 HCAPLUS
2-Naphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dimethyd-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(SCI) (CA INDEX NAME)

o/21/1-03-0 MCAPLUS
Urea, N-{4-chlorophenyl}-N'-{3-{1,1-dimethylethyl}-1-{3-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl}-1H-pyrazol-5-yl}- (9CI) (CA INDEX NAME) 872171-63-6 HCAPLUS

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

IT 872171-36-3P, 1-[5-tert-Butyl-2-[3-[[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2R-pyrazol-3-yl]-3-(naphthalen-1-yl]vrea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl]-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2R-pyrazol-3-yl]-3-[4-fluorophenyl]vrea 872171-49-8P, 1-[5-tert-Butyl-2-[3-[[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2R-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-8P, 1-[5-tert-Butyl-2-[3-[[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2R-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases) 872171-36-3 HCAPLUS CN Urea, N-[3-(1,1-dimmethylethyl)-1-[3-[[(3R)-5-[(4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Urea, N-{3-(1,1-dimethylethyl)-1-[3-{{5-[(4-methoxyphenyl)methyl]-1,1-

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-lH-pyrazol-5-yl]-n'-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

872171-49-8 HCAPLUS
Urea, N-[3-[1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}-1H-pyrazol-5-yl]-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

scaffold

AUTHOR(S):

Yue, Eddy W.; Wayland, Brian; Douty, Brent; Crawley, Matthew L.; McLaughlin, Erin; Takvorian, Amy; Wasserman, Zelda; Bower, Michael J.; Wei, Min; Li, Yanlong; Ala, Paul J.; Gonneville, Lucie: Wynn, Richard; Burn, Timothy C.; Liu, Phillip C. C.; Combs, Androw P.

CORPORATE SOURCE:

Andrew P.
Discovery Chemistry, Experimental Station, Incyte Corporation, Wilmington, DE, 19880, USA Bioorganic & Medicinal Chemistry (2006), 14(17), 5833-5849 SOURCE:

5833-5849 CODEN: BMECEP; ISSN: 0968-0896 Elsevier B.V.

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE: English

Oxo- and trioxo-substituted isothiazolidinylphenylalanines are prepared

tyrosine mimetics by Suruki coupling reactions of chloroisothiazolidinones and chlorodioxoisothiazolidinones with N-Boc-4-borono-1-phenylalanine derivs. the isothiazolidinylphenylalanines (with or without subsequent hydrogenation) are incorporated into dipeptides prepared as human protein tyrosine phosphatase 18 (PTP18) inhibitors such as I. Of the compds. tested, I is the most potent inhibitor of PTP18 with an IC50 value of 40 nM; the corresponding mixture of isothiazolidinone diastereomers inhibits PTP18 with an IC50 value of 80 nM, and the separated (R)-isothiazolidinone diastereomer inhibits PTB18 with an IC50 value of 15.5 µM; the related dispeptides prepared inhibit PTP18 less potently than either I or the mixture

mixture
of isothiazolidine diastereomers containing I. Crystal structures of a dioxothiazolidinone-substituted dipeptide and a dioxoisothiazolinone-substituted dipeptide bound to PTP1B are determined by X-ray

crystallog.; the low energy conformation found by ab initio calcus. for the saturated

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) heterocycle more closely approaches the conformation obtained upon

n PTP1B inhibitors) 850315-22-9 HCAPLUS L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-20-7P 850315-21-8P 850315-23-0P 910606-95-0P 910606-97-2P REPROPERTY OF THE PROPERTY OF

PTP1B inhibitors) 850315-20-7 HCAPLUS

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ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-21-0 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-23-0 HCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 910606-97-2 HCAPLUS
CN L-Phenylalaninamide,
L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]-N-pentyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM. 1

CRN 910606-96-1 CMF C32 H39 N5 O5 S

Absolute stereochemistry.

CM 2

CRN - 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT:

THERE ARE 39 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

910606-95-0 HCAPLUS Benzenepropanamide, α-amino-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2.5-thiadiazolidin-2-yl]-N-pentyl-, (GS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 910606-94-9 CMF C23 H30 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

L4 ANSMER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN
ED Entered STN: 07 Jul 2006
ACCESSION NUMBER: 2006:655575 HCAPLUS
DOCUMENT NUMBER: 145:124558
ITITLE: modulators
INVENTOR(S): Flynn, Daniel L.; Petillo, Peter A.
Deciphera Pharmaceuticals, LLC, USA
PCT Int. Appl., 974 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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		SG.	SK.	SL.	SM.	SY.	TJ,	TM.	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
				ZA,					-								
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		IS.	IT.	LT.	LU.	LV.	MC,	NL.	PL.	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF.	CG.	ci.	CM.	GA.	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
		GM.	KE,	LS.	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
				MD.													
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										US 2	004-	6389	86P		P 2	0041	223
										US 2						0041	

US 2004-639087P

P 20041223

OTHER SOURCE(S):

MARPAT 145:124558

The invention relates to title compds. I [A2 = bicyclic fused aryl, bicyclic fused heteroaryl, and bicyclic fused heteroaryl, etc.: A1 = pyrazolyl, Ph, pyridyl, pyrimidinyl, etc.: W, Y = CRR4, NR3 or O (wherein W and Y are not simultaneously O); X = O, S or NR3; D = Ph, heteroaryl,

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) heterocycly1, etc.; R3 = H, alky1, cycloalky1, Ph; R4 = H, alky1, hydroxyalky1, etc.) which are useful for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and diseases characterized by hypervascularization. Over 500 compds. I were prepd. E.g., a multi-step synthesis of II, starting from m-aminobenzoic acid,

given. Compds. I were tested against various kinases (ICSO values were given for representative compds. I). In a preferred embodiment, modulation of the activation state of p38 kinase protein. c-Abl kinase protein, Bcr-Abl kinase protein, Bcr-Abl kinase protein, or PDOFR kinase protein comprises the step of contacting said kinase protein with the novel compds. I.
897369-58-3P 897369-62-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea)

(preparation of pyrazolyl Ph ureas as enzyme modulators for treating

Cancer

and hyperproliferative diseases)

RN 897369-58-3 MCAPLUS

CN Ucea,
N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-3,4-dioxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-H-pyrazol-5-yl]- (9CI)

(CA INDEX NAME)

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ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) PAGE 2-A

(CA INDEX NAME)

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L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 29 Dec 2005
ACCESSION NUMBER: 2005:1346235 HCAPLUS
DOCUMENT NUMBER: 144:88279

TITLE: Preparation of 1-pyrazoly1-3-phenylurea p38 MAP kinase

inhibitors as antiinflammatory medicaments Flynn, Daniel L.; Petillo, Peter A. USA U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S. Ser. No. 746,460. CODEN: USXXCO INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

Patent English 4

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

US 200528286 A1 20051229 US 2004-886329
US 2004180906 A1 20040916 US 2003-746460
US 7144911 B2 20061205
WO 2006014290 A2 20060209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, CN, CO, CR, CU, CZ, DE, DK, DH, DZ, EC, EE, EG, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, LC, LK, IR, LS, IT, LU, LV, MA, MD, MG, MK, MN, MG, NI, NO, NZ, OM, PG, PH, PT, RO, RU, SC, SL, SM, SY, TJ, TM, TN, TT, TZ, UA, UG, US, ZA, ZM, ZW
RIAT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, IS, IT, LU, MC, M, D, EE, ES, FI, FR, CG, CI, CM, GA, CM, GQ, GW, ML, MR, NE, SN, TD, CK, KZ, ND, RU, TJ, TM
PRIORITY APPLN. INFO::

US 2003-746460 BY, ES, KM, MW, SD, U2,

US 2002-437304P

OTHER SOURCE(S): MARPAT 144:88279 1

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Title compds. (R1Xj)mA(NH)pLn(NH)pDEqYtQ [I; wherein Rl = (un)substituted (hetero)aryl; X, Y = independently O, S, NR6, NR6SO2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene,

O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h

1-4; A = (un)substituted aryl, hetero(bi)cyclyl; D = (un)substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; E = (un)substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2;

j, m, n, p, q, t = independently 0, 1; Q = $\{un\}$ substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions]

prepared as p30 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p30 kinase protein comprises the step of contacting the α -C helix, the α -D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation

not claimed, prepns. and/or characterization data for .apprx.150 examples of

and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl) acrylic acid Me ester using 10% Pd/C in EtOH provided

propionate, which was treated with NaNO2 in the presence of 6N HCl and SnCl2=2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-(3-(3-tert-butyl-5-amino-HP-pyrazole-1-yl)Phenyl)propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction with

LiOH in THF/MeOH/H2O provided the urea II. In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase

with IC50 of 45 mM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data). 872171-35-2P, 1-[5-tert-Buty1-2-[3-[[(5)-3-methyl-1,1,4-trioxo-

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-[[(R)-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-2-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) naphthalenecarboxamide 872171-62-5P, 1-(5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl}-2H-pyrazol-3-yl]-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-methoxynaphthalen-1-yllurea RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); SIOL (Biological study); PREP (Preparation); USES

(Uses)
(D38 kinase inhibitor; prepn. of (pyrazolyl)(phenyl)urea p38 kinase inhibitors as antiinflammatory agents)
872171-35-2 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-(3-[{(3S)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-37-4 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[{(3R)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

(Continued) ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-57-8 HCAPLUS 2-Naphthalenecarboxamide, N-[3-[1,1-dimethylethyl]-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (CA

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl)-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-63-6 HCAPLUS
Urea, N-{4-chlorophenyl}-N'-{3-{1,1-dimethylethyl}-1-{3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl}-1H-pyrazol-5-yl}- (9CI) (CA INDEX NAME)

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L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

IT 872171-36-3P, 1-[5-tert-Butyl-2-[3-[[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)wrea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-8P, 1-[5-tert-Butyl-2-[3-[[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of (pyrazolyl)(phenyl)urea p38 kinase inhibitors as antiinflammatory agents)
RN 872171-36-3 HCAPLUS
CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-[((3R)-5-[(4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-39-6 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(5-[(4-methoxyphenyl)methyl)-1,1-

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'(4-fluorophenyl)- (9Cl) (CA INDEX NAME)

872171-49-8 HCAPLUS
Urea, N-[3-[(1,1-dimethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-[4-fluorophenyl](9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Aug 2005 ACCESSION NUMBER: 2005:904352 HCAPLUS DOCUMENT NUMBER: 143:248386

DOCUMENT NUMBER: TITLE:

143:248386
Preparation of substituted azole derivatives for treating diseases mediated by PTPase activity Mjalli, Adnam M. M.; Polisetti, Dharma R.; Subramanian, Govindan; Quada, James C.; Arimilli, Murty N.; Yarragunta, Ravindra R.; Andrews, Robert

INVENTOR(S):

C.;

PATENT ASSIGNEE(S): SOURCE:

Xie, Rongyuan USA U.S. Pat. Appl. Publ., 204 pp. CODEN: USXXCO

DOCUMENT TYPE:

Patent English 1 LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	ENT					D	DATE					ION				ATE	
	2005						2005	0825								0050	211
AU	2005	2143	49		A1		2005	0901		AU 2	005-	2143	49		2	0050	211
CA	2551	909			A1		2005	0901		CA 2	005-	2551	909		2	0050	211
wo	2005	0803	46,		A1		2005	0901		WO 2	005-	US 45	90		2	0050	211
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC.	EE,	EG,	ES,	FI,	GB,	GD
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	FC
		LK,	LR.	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NA,	NI
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	υG,	US,	UZ,	V¢,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	М2,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK
		EE,	ES,	FI,	FR,	GB,	GR,	Hυ,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML
					TD,												
EP	1730	118			A1		2006	1213		EP 2	005-	7230	26		2	0050	211
	R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	ĐΚ,	ÉΕ,	ÉS,	FI,	FR,	GB,	GR,	ΗU,	ΙE
		IS,	IT,	LI,	LT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	AL,	BA
		HR,	LV,	MK,	YU												
RIT	APP	LN.	INFO	.:						US 2	004-	5439	71P		P 2	0040	212

WO 2005-US4590 W 20050211

MARPAT 143:248386

$$T \xrightarrow{L^2 \cdot Ar^2 \xrightarrow{L^1} \xrightarrow{M} \xrightarrow{N} = N} Ar^1$$

AB The title compds. I [a, b = 0-2; W = 0, 5, NR2 (wherein R2 = alkyl, etc.); R1 = H, halo, CN, etc.; L1 = a direct bond, (un)substituted NHCO, NHSO2,

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
etc.; Ar1 = (un)substituted (hetero)arylene, fused cycloalkylaryl, etc.; Ar2
= (un)substituted (hetero)arylene, fused arylcycloalkylaryl, etc.; L2 =
CH2, O, alkylene, etc.) which can be useful as inhibitors of protein
tyrosine phosphatases and thus can be useful as inhibitors of protein
tyrosine phosphatases and thus can be useful as inhibitors of protein
tyrosine phosphatases and thus can be useful for the management,
treatment, control, or the adjunct treatment of diseases mediated by
PTPase activity such as type I diabetes and type II diabetes, were prepd.
Thus, treating
-{2,4-dichlorophenyl}-2-(2-(4-methoxyphenyl)-(E)-vinyl]-1Himidazole with Me bromoacetate followed by ester hydrolysis afforded 56%
[4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1H-imidazol-1yl]acetic acid. The representative compds. I were tested for inhibition
of PTP-1B. In general, the exemplified compds. I may inhibit PTP-1B with
IC50 of less than 20 µM. The pharmaceutical compns. comprising the
compds. I, and their use in treating human or animal disorders are also
disclosed.

I 862243-91-98 863245-57-2P 863245-74-3P
-862246-05-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); TRU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted arole derivs. for treating diseases
mediated by PTPase activity)
RN 863243-91-8 HCAPLUS

N1, 2, 5-Thiadiazolidin-3-one, 5-(4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'(trifluoromethyl.]), 1, 1'-biphenyl]-4-y-l]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-4, 4-dimethyl-, 1, 1-dioxide (SCI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

863243-80-5p 863243-92-9p 863243-93-0p 863243-94-1p 863244-05-7p 863244-06-6p 863244-07-p9 863244-08-7p 863244-17-8p 863244-51-7p 863244-17-8p 863244-51-7p 863244-51-7p 863244-51-5p 863245-51-4p 863245-55-1p 863245-55-1p 863245-56-1p 863245-56-1p 863245-56-1p 863245-56-1p 863245-66-1p 863245-60-1p 863245-60-1p 863245-60-1p 863245-60-1p 863246-00-2p 863246-00-2p 863246-00-863246-11-1p 863246-10-9p 863246-11-1p 863246-10-9p 863246-11-1p 863246-10-9p 863246-11-1p 863246-10-6p 863246-11-1p 863246-10-6p 863246-11-1p 863246-11-6p 863246-16-6p 863247-00-1p 863246-11-1p 863246-16-5p 863246-16-6p 863247-00-1p 863246-11-1p 863246-16-5p 863246-16-6p 863247-00-1p 863246-10-1p 863246-16-6p 863246-16-6p 863246-16-6p 863246-10-1p 863246-16-6p 863246-1

B0328;-U3-UF RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of substituted azole derivs. for treating diseases mediated by PTPase activity)
RN 863243-80-5 MCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[(4-(2,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

863245-74-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl)phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:Benzoic acid} $$Benzoic acid, $$4-[4-(2,4-dichlorophenyl)-2-[\{1E\}-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME) $$.$$$

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863243-92-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-2,4,4-trimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863243-93-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-phenyl-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 863243-94-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2-chlorophenyl)-2-((1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-06-8 HCAPLUS

N 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-07-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoropethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863243-95-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(4-chlorophenyl)-2-[(1E)-2-[3'-(triffluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-05-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-08-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2-chloro-4-fluorophenyl)-2-[(1E)-2[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-13-7 HCAPLUS
CN 1,2,5-Thisdiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[[3'(methylsulfonyl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazol-1-yl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-51-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[2-[4-

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-53-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[2-[3'-(trifluoromethoxy](1,1'-bipheny1]-4-y1]ethy1]-1H-imidazol-1-y1]methy1]pheny1}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-25-4 HCAPLUS CN Benzoic acid, 4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxoL4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued) (trifluoromethyl)phenyl)ethyl)-1H-imidazol-1-yl]methyl]phenyl)-, l,1-dioxide (9C1) (CA INDEX NAME)

RN 863244-52-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[4-(2,4-dichlorophenyl)-2-[2-[2-fluoro-4(trifluoromethyl)]henyl]ethyl]-lH-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-iH-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-56-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[(2-[(1E)-2-[3',5'-bis(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-4-(2,4-dichlorophenyl)HH-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-58-3 HCAPLUS
1,2,5-Thiaddazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(2'-fluoro-5'-propoxy[1,1'-biphenyl]-4-yl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

14 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-{(1E)-2-{3'-chloro[1,1'-biphenyl]-4-y1}ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-y1]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-60-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(1-

methylethoxy){1,1'-biphenyl}-4-yl}ethenyl}-1H-imidazol-1-yl}methyl}phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Double bond geometry as shown.

RN 863245-63-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dimethylethyl)-5'-methyl[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-64-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-[[1E]-2-[4-[5-chloro-2-thienyl]phenyl]]ethenyl]-4-[2,4-dichlorophenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-61-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4'[(1-methylethyl)thio][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidezol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-62-9 HCAPLUS
(1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]ethenyl]-lH-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continu

RN 863245-66-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-[(1E)-2-[4-(5-acetyl-2-thionyl)phenyl]ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-67-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2'-fluoron-5'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (SCI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-68-5 HCAPLUS
1,2,5-Thiadkazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(3,3-dimethylbutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

Double bond geometry as shown.

863245-69-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(4,4,4-trifluorobutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

863245-72-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-75-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]2-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-70-9 RCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-

fluoro-4'-{4,4,4-trifluorobutoxy}{1,1'-biphenyl}-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA-INDEX NAME)

Double bond geometry as shown.

863245-71-0 HCAPLUS
Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl]-4-fluoro[1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863245-78-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4-(4,4,4-trifluorobutoxy)phenyl]-thenyl]-lH-imidazol-1-yl}methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-80-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-{2,4-dichlorophenyl}-2-[(1E)-2-[4-[4-

(1,1-dimethylethyl)phenoxy]phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-82-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[4-[4-

(trifluoromethyl)phenoxy]phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-{(1E)-2-[3'(methylsulfonyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

RN 863246-09-7 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1-2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Double bond geometry as shown.

RN 863246-04-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-{(1E)-2-[4-(2,4-dichlorophenyl)-1-ethyl-1H-imidazol-2-yl]ethenyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-06-4 HCAPLUS
CN Benzoic acid, 4-[{4-(2,4-dichlorophenyl)-2-{{1E}-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethenyl}-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 863246-10-0 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-11-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[[4-(2,4-dichlorophenyl)-2-[(18)-2-[3'-(1-

methylethyl) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

863246-13-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-phenoxyphenyl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide

(CA INDEX NAME) Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

Double bond geometry as shown.

IT 863247-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Reactant or reagent)
mediated by
PTPase activity)
RN 863247-41-0 HCAPLUS
CN Benzoic acid,
4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo-

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-15-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-

(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-2-methylphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:continuous} $863246-16-6$$$ HCAPLUS $1,2,5-Thiadiazolidin-3-one, $5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(3'-trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-propyl-, 1,1-dioxide (9CI) (CA INDEX NAME)$

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 03 May 2005 ACCESSION NUMBER: 2005:378875 HCAPLUS DOCUMENT NUMBER: 143:19267 HCAPLUS Structure-based design of protein and protein access to the state of the

ACCESSION NUMBER: 2005;378875 HCAPLUS
DOCUMENT NUMBER: 143:19267

AUTHOR(S): Structure-based design of protein tyrosine phosphatase-18 inhibitors

AUTHOR(S): Black, Emma: Breed, Jason; Breeze, Alexander L.; Embrey, Kevin; Garcia, Robert; Gero, Thomas W.; Godfrey, Linda; Kenny, Peter W.; Morley, Andrew D.; Minshull, Claire A.; Pannifer, Andrew D.; Read, Jon; Rees, Amanda; Russell, Daniel J.; Toader, Dorin; Tucker, Julie

CORPORATE SOURCE: AstraZeneca, Cheshire, SK10 4TG, UK
BOURCE: Bioorganic 4 Medicinal Chemistry Letters (2005), 15(10), 2503-2507

CODEN: BMCLBS; ISSN: 0960-894X

PUBLISHER: DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 143:19267

AB Using structure-based design, a new class of inhibitors of protein tyrosine phosphatase-18 (PPTB) has been identified, which incorporate the

1,2,5-thiadiarolidin-3-one-1,1-dioxide template.
692765-80-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-based design of protein tyrosine phosphatase-1B inhibitors)
692765-80-3 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-44-6P 692764-89-9P 692764-94-6P
852835-44-0P 852835-45-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(structure-based design of protein tyrosine phosphatase-1B inhibitors)
612530-44-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852835-45-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT: THIS

THERE ARE 22 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-89-9 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

692764-94-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-bipheny1]-3-y1-, 1,1-dioxide (9CI) (CA INDEX NAME)

852835-44-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2005
ACCESSION NUMBER: 2005:347030 HCAPLUS
DOCUMENT NUMBER: 142:411350

ITILE: Preparation of 1-oxo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins

Combs, Andrew P.; Yue, Eddy Wai Taun; Bower, Michael Jason; Zhu, Wenyu; Crawley, Matthew Lentz; Sparks, Richard Bruce; Pruitt, James Russell; Takvorian, Amy

PATENT ASSIGNEE(S): CODEN: PIXKD2

POCUMENT TYPE: LANGGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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		CN,	co,	CR,	Cυ,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
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CASREACT 142:411350; MARPAT 142:411350

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention provides 1-oxo and 1,1-dioxoisothiazolones (shown

I-IV; also isothiazolidinone analogs of I-IV with R16 and R17 in place of R15 and Rz as a substituent at the 5 position of the isothiazolidinone ring; variables defined below; e.g. V) and related compds. that can modulate (no data) the activity of a target protein, such as a phosphatase, that selectively binds phosphorylated peptides or proteins. The present compds. can be useful (no data) in treating diseases or disorders, including, for example, diabetes and obesity, that are connected directly or indirectly to the activity of the target protein. Methods of preparation are claimed and hundreds of example prepns. are included. For example, V was prepared in 12 steps (50, 62, 100, 59, not

- ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) detd., 100, 100, 99, not detd., not detd., 43, and 25 % yield) starting from N-tert-butyl-3-[2-(tert-butylcarbamoyl)ethyldisulfanyl]propionamide. For I-TV: a dashed line indicates an optional bond; Scl is a 1st mol. scaffold or is absent; Sc2 is a 2nd mol. scaffold or is absent, wherein
- least one of Sc1 and Sc2 is present; or Sc1 and Sc2 together with X1 and X2 or X4 and X5 form a 5-, 6-, or 7-membered fused carbocyclic ring or a 5-, 5-, or 7-membered fused heterocarbocyclic ring; X1 is C or N when Sc1 is present; X1 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc1 is absent; X2 is C or N when Sc1 is present; X2 is C or N when Sc2 is present; X2 is C or N when Sc2 is present; X2 is C or N when Sc2 is present; X2 is C or N, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2, wherein the ring formed by X1, X2, X3, D1, D2, and D3 is an arom. ring; X4 is C or N when Sc1 is present; X4 is O, S, CR3, N, NR4,
- CS, SO, or SO2 when Sc1 is absent; X5 is C or N when Sc2 is present; X5
- O, S, CR3, N, NR4, CO, CS, SO, or SO2 when Sc2 is absent; X6 is C or N. Each E1 and E2 = O, S, CR3, N, NR4, CO, CS, SO, or SO2, wherein the rin formed by X4, X5, X6, E1, and E2 is an aron. ring; Rz is H, halo, C1-C4 alky1, C3-C6 cycloalky1, haloalky1, OR28, SR28, NO2, CN, SOR29, SOR29, COR30, COR031, NR32R33, a 5 or 6-bembered heterocarbocycly1 group, or tetrazoly1. R15 is H, halo, C1-C4 alky1, C3-C6 cycloalky1, haloalky1,
- tetrazolyl. R15 is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl, OH,

 C1-C4 alkoxy, C1-C4 haloalkoxy, SH, C1-C4-chioalkoxy, CN, NO2, SO(C1-C4 alkyl), SO(C1-C4 haloalkyl), SO(C3-C6 cycloalkyl), SO(R2, SO3H, SO2(C1-C4 alkyl), SO(C1-C4 haloalkyl), SO(C1-C6 alkyl), SO2(C1-C4 haloalkyl), C0(C1-C6 cycloalkyl), SO2(R12, CHO, COOH, C0(C1-C4 alkyl), CO(C1-C4 haloalkyl), CO(C1-C4 haloalkyl), CO(C1-C4 haloalkyl), CO(C1-C4 haloalkyl), CON(C1-C4 cycloalkyl), CON(C1-C4 alkyl), CON(C1-C4 alkyl), CON(C1-C4 alkyl), CON(C1-C4 alkyl), N(C1-C4 alkyl), SO(C1-C4 alkyl), CO(C1-C4 alkyl),

- Retailsolytiolarly years. In the collains.

 850315-19-4P, [(1S)-1-[{(1S)-1-{Pentylcarbamoyl}-2-[4-{1,1,4-trioxo[1,2,5]thiadiacolidin-2-yl]phenyl]ethyl]carbamoyl]-2-phenylethyl]carbamic acid tert-butyl ester 850315-22-9P, (2S)-2-[(2C)-2-[(2-(4-Methoxyphenyl)acetyl]amino]-3-
- phenylpropionyl]amino]-N-pentyl-3-{4-{1,1,4-trioxo[1,2,5}thiadiazolidin-2-yl]phenyl]propionamide 850315-24-1P, N-{(15)-2-{4-(1,1-Dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]biphenyl-4-sulfonamide 850315-36-59 850315-40-1P, 4-Bromo-N-{(15)-2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-
- ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 850327-93-4P, N-[(15)-1-(1H-Benzimidazol-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3-chlorobenzenesulfonamide trifluoroacetate 850327-95-6P, N-[(15)-1-(1H-Benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3-fluorobenzenesulfonamide trifluoroacetate
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); TNU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 - (drug candidate; prepn. of 1-oxo and 1,1-dioxoisothiazolone and
- related
- modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins)
 85-015-19-4 MCAPLUS
 85-015-19-4 MCAPLUS
 (1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- 850315-22-9 HCAPLUS L-Phenylalaninanide, N-{(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- 850315-24-1 HCAPLUS
 [1,1'-Biphenyl]-4-sulfonamide, N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

- ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 550315-44-5p, N-{(15)}-2-{4-(1,-1)coxid-4-caxc-1,2,5-chiadizarolidin-2-yl)phenyl}-1-{5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 550315-48-9p, N-{(15)}-2-{4-(1,-1)coxid-4-caxc-1,2,5-chiadizzolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxyl)benzenesulfonamide trifluoroacetate 550315-63-py, N-{(15)}-2-(3-chiadizzolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]biphenyl-4-sulfonamide trifluoroacetate 850315-65-0P 850315-69-4P
- 4-Bromo-N-[(15)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-73-0P, N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 850327-65-0P 850327-67-2P, N-[(15)-1-{5-Chloro-1H-
- benzimidazo1-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-69-49, N-[(15)-1-(5-Chloro-lH-benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-71-89,
- N-[(1S)-1-(5-Chloro-1H-benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 650327-73-0P, N-[(1S)-1-(5-Chloro-1H-
- benzimidasol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)phenyl)ethyl)-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-75-2P, N-[(15)-1-(5-Chloro-1H-benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-77-4P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-79-6P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-83-2P, N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-83-2P, N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide
- 2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-85-4P,
 N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3, 4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-5P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-89-8P,
 3-Chloro-N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-91-2P, N-[(1S)-1-(5-chloro-1H-
- benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-fluorobenzenesulfonamide trifluoroacetate

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- RN 850315-36-5 HCAPLUS
 CN Benzenesulfonanide,
 y1[t3]-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl]-4(trifluoromethyl)-, monotrifluoroacetate) 9C1) (CA INDEX NAME)

 - CRN 850315-35-4 CMF C25 H19 F6 N5 O5 S2
- Absolute stereochemistry.

- CM 2
- CRN 76-05-1 CMF CZ H F3 O2

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)

850315-40-1 HCAPLUS
Benzenesulfonamide, 4-bromo-N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-39-8 CMF C25 H18 Br F6 N5 O6 S2

Absolute stereochemistry.

RN 850315-44-5 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-63-8 HCAPLUS
[1,1'-Biphenyl]-4-sulfonamide, N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-

1,2,5-thiadiarolidin-2-yl)phenyl}-1-{5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl}-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-62-7 CMF C30 H23 C1 F3 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bia(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-43-4 CMF C26 H18 F9 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

Absolute stereochemistry.

RN 850315-48-9 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2(trifluoromethoxy)-, mono(trifluorometate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-47-8 CMF C25 H19 F6 N5 O6 S2

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 2

-со2н

850315-65-0 HCAPLUS
Benzenesulfonamide, N-[(1S)-2-[3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1R-benzimidazol-2-yl]ethyl]-4-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-64-9 CMF C25 H18 C1 F6 N5 O5 S2

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- со2н

RN 850315-69-4 HCAPLUS
CN Benzenesulfonamide,
4-bromo-N-[(15)-2-[3-chloro-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-[trifluoromethyl]-1H-benzimidazol-2-yl]ethyl]-2-[trifluoromethoxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

См 1-

CRN 850315-68-3 CMF C25 H17 Br C1 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-65-0 HCAPLUS

Benzenesulfonamide,
N-{(iS)-1-{S-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-4-(l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenyl]ethyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-64-9 CMF C23 H19 C12 N5 O5 52

Absolute stereochemistry.

CM 2

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 02

850315-73-0 HCAPLUS Benzenesulfonanide, N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-72-9 CMF C26 H17 C1 F9 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-67-2 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-1-(5-chloro-lH-benzimidazol-2-yl)-2-{3-chloro4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-2-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-66-1 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

RN 850327-69-4 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-1-{5-chloro-lH-benzimidazol-2-yl}-2-{3-chloro4-{1,1-dioxido-4-oxo-1,2,5-chliadiazolidin-2-yl}phenyl]ethyl}-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 1

CRN 850327-68-3 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-71-8 HCAPLUS
CN Benzeneaulfonamide,
f([X]s)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxy-,
mono(cirfluoroacetate) [9CI) (CA INDEX NAMES)

CM 1

CRN 850327-70-7 CMF C29 H23 C12 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-75-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-74-1 CMF C25 H23 C12 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 850327-73-0 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-3,4-dimethoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-72-9 CMF C25 H23 C12 N5 O7 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-77-4 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-76-3 CMF C23 H20 C1 N5 O5 S2

Absolute stereochemistry.

CRN 76-05-1

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CMF C2 H F3 O2 (Continued)

850327-79-6 HCAPLUS
Benzenesulfonamide, N-[(18)-1-(1H-benzimidazo1-2-y1)-2-[3-chloro-4-(1,1-dioxido4-4-oxo-1,2,5-thiadiazolidin-2-y1]phenyl]ethyl]-2-cyano-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-78-5 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

2

850327-81-0 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-vox-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-, mono(trifluoroacetate) {9CI} {CA INDEX NAME}

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

СМ

850327-85-4 HCAPLUS
Benzenesulfonamide, N-{(1S)-1-{1H-benzimidazol-2-yl}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl]phenyl]ethyl]-3,4-dimethoxy-,
mono(trifluoroacetate) (9CI) {CA INDEX NAME}

CRN 850327-84-3 CMF C25 H24 C1 N5 O7 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM 1

CRN 850327-80-9 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-83-2 HCAPLUS
Benzenesulfonamide, N-{(15)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxy-, mono(trifluoroacetate) (9CI) {CA INDEX NAME}

CRN 850327-82-1 CMF C29 H24 C1 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850327-87-6 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2;yl)phenyl]ethyl]-3,5-dimethyl-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-86-5 CMF C25 H24 C1 N5 O5 S2

Absolute stereochemistry.

CM 2

850327-89-8 HCAPLUS
Benzenesulfonamide, 3-chloro-N-[(1s)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)phenyl]ethyl]-,

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN mono(trifluoroacetate) (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 850327-88-7 CMF C23 H18 C13 N5 O5 S2

Absolute stereochemistry.

см 2

CRN 76-05-1 CMF C2 H F3 O2

850327-91-2 HCAPLUS
Benzenesulfonamide,
[13]-1-[5-chloro-IH-benzinidazol-2-yl]-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]ethyl]-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-90-1 CMF C23 H18 C12 F N5 O5 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

-CO2H

850327-95-6 HCAPLUS

Benzenesulfonamide, N-{{15}-1-{1H-benzimidazo1-2-y1}-2-{3-chloro-4-{1,1-dioxido-4-xoc-1,2,5-chiadiazolidin-2-y1}pheny1}ethy1}-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-94-5 CMF C23 H19 Cl F N5 OS S2

Absolute stereochemistry.

1.4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-93-4 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazo1-2-y1)-2-[3-chloro-4-(1,1-dioxido4-4-oxo-1,2,5-chiadiazolidin-2-y1]phenyl]ethyl]-3-chloro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-92-3 CMF C23 H19 C12 N5 O5 52

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM $\,$ 2

CO2H

IT 850315-20-7P, [(5)-2-[4-(5-Benzyl-1,1,4-

IT 850315-20-7P, {(5)-2-(4-(5-Benzyl-1,1,4trioxo(1,2,5)thiadiazolidin-2-yl)phenyl]-1-(pentylcarbamoyl)ethyl]carbamic
acid tert-butyl ester 850315-21-8P, {(15)-1-[(15)-2-(4-(5Benzyl-1,1,4-trioxo(1,2,5)thiadiazolidin-2-yl)phenyl]-1(pentylcarbamoyl)ethyl]carbamoyl]-2-phenylethyl]carbamic acid tert-butyl
ester 850315-23-0P, {25)-3-[4-(5-Benzyl-1,1,4trioxo(1,2,5)thiadiazolidin-2-yl)phenyl]-2-[(25)-2-[(2-(4methoxyphenyl)acetyl]amino]-3-phenylpropionyl]amino]-N-pentylpropionamide
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation of 1-oxo and 1,1-dioxoisothiazolone and related
modulators of

proteins such as phosphatases that bind phosphorylated peptides and
proteins)
RN 850315-20-7 HCAPLUS
CArbamic acid, ([15)-1-[[4-[1,1-dioxido-4-oxo-5-(phenylmethyl]-1,2,5thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

850315-21-8 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-23-0 HCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612528-23-1P 612529-46-1P 612530-69-5P
82328-50-0P 852358-51-1P 852358-53-3P
852358-54-4P 852358-56-6P 852358-57-7P
RL: SPN (Synthetic preparation) PREP (Preparation)
(preparation of sulfonylhydantoins via reaction of amino acid esters

sulfamide and DBU) 612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2-CH2-Ph

612529-46-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2-bromophenyl)methyl}-, 1,1-dioxide {9CI}(CA INDEX NAME)

612530-69-5 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN CN (9CI) 852358-50-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-, 1,1-dioxide (CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 11 Apr 2005 ACCESSION NUMBER: 2005:308290 HCAPLUS DOCUMENT NUMBER: 143:7658

DOCUMENT NUMBER: TITLE:

143:7658
Expedient syntheses of sulfonylhydantoins and two
six-membered analogs
Campbell, Andrew D.; Birch, Alan M.
Research and Development, AstraZeneca, Cheshire, SK10

AUTHOR(S): CORPORATE SOURCE:

Research and Development, Astra 4TC, UK Synlett (2005), (5), 834-838 CODEN: SYNLES; ISSN: 0936-5214 Georg Thieme Verlag Journal English CASREACT 143:7658 SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

A range of α -amino esters can be turned into sulfonylhydantoins in a single, atom-economic step using sulfamide and DBU. E.g., reaction of BRHNCH2CO2Ct with sulfamide and DBU gave 65% sulfonylhydantoin I. This procedure obviates the need for a three- or four-step sequence utilized

traditional procedures. Two new six-membered analogs [5-aryl-1,2,6-thiadiazinan-3-one 1,1-dioxides and 5-aryl-1,2-thiazinan-3-one 1,1-dioxides), e.g. II and III, have also been prepared utilizing novel synthetic protocols.

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-51-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{2-methoxyphenyl}methyl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

852358-53-3 HCAPLUS
Benzonitrile, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)(9CI) (CA INDEX NAME)

852358-54-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,ethyl ester (9CI) (CA INDEX NAME)

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-56-6 HCAPLUS 1,2,5-Thiediarolidin-3-one, 5-([1,1'-biphenyl]-3-ylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

852358-\$7-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-methyl-5-(phenylmethyl)-, 1,1-dioxide, (45) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 08 Mar 2005 ACCESSION NUMBER: 2005:202894 HCAPLUS DOCUMENT NUMBER: 142:366767 TITLE: 1.2 5. mc// ...

ACCESSION NUMBER: 2005:202894 HCAPLUS
DOCUMENT NUMBER: 142:366767

ITILE: 12:366767

ITILE: heterocyclic sulfides are potent inhibitors of human tryptase
AUTHOR(S): Wong, Tzutshin: Groutas, Christopher S.: Mohan, Swathi; Lai, Zhong; Alliston, Kevin R.: Yu, Nga: Schechter, Norman M.: Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Archives of Biochemistry and Biophysics (2005), 436(1), 1-7
CODEN: ABBIAA; ISSN: 0003-9861

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors describe herein the design, synthesis, and in vitro biochem. evaluation of a series of potent, time-dependent inhibitors of the mast cell-derived serine processe tryptase. The inhibitors were readily obtained by attaching verious heterocyclic thiols, as well as a basic primary specificity residue Pl. to the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold. The inhibitors were found to be devoid of any inhibitory activity toward a neutral (elastase) or cysteine (papain) protease, however they were also fairly efficient inhibitors of bovine trypain. The differential inhibition observed with trypain suggests that enzyme selectivity can be optimized by exploiting differences in the S' subsites of the two enzymes. The results described herein demonstrate the

versatility of the heterocyclic scaffold in fashioning mechanism-based inhibitors of neutral, basic, and acidic (chymo)trypsin-like serine

Innoltors of neutral, basic, and actiff (clipmo) trypoin fine Series Proteases. 849415-30-1P 849415-31-2P 849415-32-3P REPORT (Pheramacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES IT

(1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides are

potent inhibitors of human tryptase)
849415-30-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-2-[(2-benzoxazolylthio)methyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-31-2 KCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-({(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

849415-32-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{4-aminobutyl}-5-{phenylmethyl}-2-{{(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl}-, 1,1-dioxide, (45)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

849415-24-3P 849415-25-4P 849415-26-5P 849415-27-6P 849415-28-7P 849415-29-8P RL: RCT (Reactant); SPR (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

potent inhibitors of human tryptase)
849415-24-3 RCAPLUS
Carbamic acid, [4-{(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

849415-25-4 HCAPLUS
Carbamic acid, (4-((33)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5[(phenylthio]methyl]-1,2,5-thiadiazolidin-3-yl]bucyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-26-5 HCAPLUS
Carbamic acid, {4-[(33)-5-(chloromethyl)-1,l-dioxido-4-oxo-2-(phenylmethyl)-1,2,5-thladiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 849415-27-6 HCAPLUS
CN Carbamic acid,
[4-[(35)-5-([2-benzoxazolylthio]methyl]-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

THERE ARE 32 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

849415-28-7 HCAPLUS
Carbamic acid, {4-[(33)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5-[[(5-phenyl-1,3,4-oxdiazol-2-yl)thio]methyl]-1,2,5-thiadiazolidin-3-yl}butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

849415-29-8 HCAPLUS
Carbamic acid, {4-[(33)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5-[[(3-phenyl-1,2,4-oxdiazol-5-yl)thio]methyl)-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 19 Aug 2004 ACCESSION NUMBER: 2004:677210 HCAPLUS 2004:677210 RCAPLUS
141:23569
Potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin-3-one 1,1 dioxide-based
sulfonamide derivatives
Lai, Zhong; Gan, Xiangdong; Wei, Liuqing; Alliston,
Kevin R.; Yu, Hongyl; Li, Yue H.; Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, XS, 67260, USA
Archives of Biochemistry and Biophysics (2004),
429(2), 191-197
CODEN: ABBIA4; ISSN: 0003-9861
Elsewier
Journal DOCUMENT NUMBER: TITLE: AUTHOR (S): CORPORATE SOURCE: SOURCE: PUBLISHER: Journal English CASREACT 141:235669 DOCUMENT TYPE: OTHER SOURCE(S):

CASREACT 141:235669

AB The design, synthesis, and in vitro biochem. evaluation of a class of mechanism-based inhibitors of human leukocyte elastase (HLE) that incorporate in their structure a 1,2,5-thiadiazolidin-1-one 1,1-dioxide scaffold with appropriate recognition and reactivity elements appended to it is described. The synthesized compds, were found to be efficient, time-dependent inhibitors of HLE. The interaction of the inhibitors with HLE is postulated to lead to the formation of a highly reactive N-sulfonyl imine (a Michael acceptor) that arises from an enzyme-induced sulfonamide fragmentation cascade. Subsequent reaction ultimately leads to the formation of a relatively stable acyl enzyme. The results cited herein demonstrate convincingly the superiority of the 1,2,5-thiadiazolidin-1-one
1,1 dioxide scaffold over other scaffolds (e.g., saccharin) in the design OTHER SOURCE(S): li dioxide scaffold over other scaffolds (e.g., saccharin) in the design of inhibitors of (chymoltryppin-like serine proteases. 749866-31-79 749866-32-89 749866-33-99 749866-40-0P 749866-34-0P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Proparation); USES (Usea) (potent inhibition of human leukocyte elastase by 1,2,5-thiadiarolidin-3-one 1,1-dioxide-based sulfonamide derivs.)
RN 749866-31-7 HCAPLUS
CN L-Phenylalanine, N-[[[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-32-8 HCAPLUS D-Phenylalanine, N-[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM (Continued) (phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-33-9 HCAPLUS
L-Phenylalanine, N-{[{(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-34-0 HCAPLUS
L-Phenylalanine, N-[{[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl]sulfonyl]- (9CI) INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 212331-99-2P 749866-30-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin-

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT: THIS

THERE ARE 36 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 3-one 1,1-dioxide-based sulfonamide derivs.)
212331-99-2 HCAPLUS (2006)
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)-[9CI] (CA INDEX NAME) L4 (Continued)

Absolute stereochemistry.

749866-30-6 HCAPLUS Ethanethioic acid, S-[{{4S}-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester {9CI} (CA INDEX NAME)

Absolute stereochemistry.

IT 220869-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
{potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.}
RN 220869-64-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 30 Jul 2004

ACCESSION NUMBER: 2004:610081 HCAPLUS

DOCUMENT NUMBER: 141:157120

TITLE: Preparation of sulfahydantoins as phosphate isosteres for use as phosphatase inhibitors in the treatment of cancer and autoimmune disorders

INVENTOR(5): Saunders, Jeffrey O.; Miknis, Gregory F.; Blake, James

INVENTOR(5):

F. Vertex Pharmaceuticals Incorporated, USA PCT Int. Appl., 62 pp. CODEN: PIXXD2 Patent English 1 PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

											LICAT					ATE	
											2003-					0031	230
	W:										, BG,						
											, EE,						
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	, KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT.	LU,	LV,	MA,	MD,	MG,	MK,	MN,	, MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	Rυ,	SD,	SE,	SG,	SK,	SL	, TJ,	TM,	TN,	TR,	ΤT,	TZ,	UA,
		UG,	US,	UΖ,	VN,	YU,	ZA,	2M,	2W								
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL	, 52,	TZ,	UG,	ZM,	ZW,	AM,	AZ,
		BY,	KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	AT,	BE	, BG,	CH,	CY,	cz,	DΕ,	DK,	EE,
		ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU	, MC,	NL,	PT,	RO,	SE,	SI,	SK,
		TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN.	, GQ,	GW,	ML,	MR,	NE,	SN,	TD,
TG																	
CA	2511	818			A1		2004	0729		CA :	2003-	2511	818		2	0031	230
											2003-						
US	2004	1671	87		A1		2004	0826		US :	2003-	7491	21		2	0031	230
EP	1594	497			A1		2005	1116		EP :	2003-	8152	58		2	0031	230
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL	, TR,	BG,	CZ,	EE,	HU,	sĸ	
											2004-						
PRIORIT	Y APP	LN.	INFO	.:						ŲS :	2002-	4375	72P		P 2	0021	230
										wo :	2003-	US41	630		W 2	0031	230

OTHER SOURCE(S): MARPAT 141:157120

1.4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

The invention relates to compds. having a sulfahydantoin or a reverse sulfahydantoin moiety (I) and (II) or pharmaceutically acceptable salts thereof (Q = each (un)substituted Cl-8 aliphatic group, C6-10 aryl, heteroaryl having 3-10 ring atoms, heterocyclyl having 3-10 ring atoms, recorded to the control of the control

nitrogen are taken together with the nitrogen to form a 3-7 membered heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen,

heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen, wherein said heteroatoms are independently selected from N, O, or S], uses thereof, and related methods. These compds. are inhibitors of phosphatases, particularly inhibitors of protein tyrosine phosphatase SHP-2 and are used in the treatment of various phosphatase mediated diseases such as proliferative diseases, autoimmune disorders, angiogenic disorders, and cancer. The autoimmune disease is selected from glomerulonephritis, rheumatoid arthritis, systemic lupus erythematosus, scleroderma, chronic thyroiditis, Graves' disease, autoimmune sastritis, diabetes, autoimmune hemolytic anemia, autoimmune neutropenia, thrombocytopenia, atopic dermatitis, chronic active hepatitis, myasthenia gravis, multiple sclerosis, inflammatory bowel disease, ulcerative colitis, Crohn's disease, psoriasis, or graft vs. host disease. The proliferative disease is selected from acute myelogenous leukemia, chronic myelogenous leukemia, metastatic melanoms.

prouiterative disease is selected from acute myelogenous leukemia, mic myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple myeloma, and HTLV-1-mediated tumorigenesis. The angiogenic disorder is selected from solid tumors, ocular neovasculization, and infantile haemangiomas. The cancer is selected from colon, breast, stomach, and ovarian cancer. Thus, N-alkylation of Me 4-aminobenzoate by Et bromoacetate in the presence of EIN at 60° for 2.5 days gave 4-[[Ethoxycarbonyl]methyl]amino]benzoic acid Me ester which underwent N-aulfamoylation by aulfamoyl chloride in the presence of EIN in CHZC12 at room temperature overnight to give 4-[N-[Ethoxycarbonyl]methyl]-N-sulfamoylamino]benzoic acid Me ester [III]. Cyclization of III by treatment with NaOMe/MeON at room temperature overnight gave 4-(1,1,4-tricxo-1,2,5-thiadiszolidin-2-yl)benzoic acid Me ester (IV). IV showed ICSO of 1.0-1.00 µM against protein tyrosine phosphatase SHP-2. 612527-99-8P 612530-69-SP 729600-44-6F,

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

729600-47-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenyl)-, 1,1-dioxide (9CI) (CA

729600-48-0 HCAPLUS Benzoic acid, 3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-, methyl ester (9CI) (CA INDEX NAME)

729600-49-1 HCAPLUS
1,2,5-Thiediarolldin-3-one, 5-(3-phenyl-2-propenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 4-(1,1,4-Trioxo-[1,2,5]thiadiazolidin-2-yl]benzoic acid methyl ester 729600-47-9P 729600-48-0P 729600-49-1P 729600-50-5P 729600-51-5P 729600-52-6P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (prepn. of sulfahydantoins as phosphate isosteres for use as protein

phosphatase inhibitors in treatment of cancer and autoimmune . disorders) rders) 612527-99-8 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, methyl ester (9CI) (CA INDEX NAME)

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-44-6 HCAPLUS
Benzoic acid, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
ester (9C1) (CA INDEX NAME)

(Continued) ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

729600-50-4 HCAPLUS Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

729600-51-5 HCAPLUS
Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

729600-52-6 HCAPLUS Benzamide, N-butyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Sulfamides, such as I, were prepared for use as anticancer agents which

by modulating the activation states of abl or bcr-abl α -kinase proteins. Thus, 4-H02CC6H4CH2NH5O3NHCOR [R = pyrrolidino], prepared from 4-Me02CC6H4CH2NH2 and pyrrolidine, was treated with the pyrimidinylaminoaniline fragment to give I, which showed 10% inhibition

non-phosphorylated abl kinase at 10µM.
726192-44-5P 726192-45-6P 726192-60-5P
726192-61-6P
RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of sulfamides as anti-cancer agents)
726192-44-5 HCAPIUS
Benzamide, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 23 Jul 2004
ACCESSION NUMBER: 2004:589375 HCAPLUS
141:140459
TITLE: 1NVENTOR(S): Preparation of sulfamides as anti-cancer agents
Flynn, Daniel L.: Petrillo, Peter A.
Deciphera Pharmaceuticals, Inc., USA
PCT Int. Appl., 168 pp.
CODENT TYPE: Patent

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT	NO.	KIND	DATE	APPLICATION NO.	DATE
				WO 2003-US41425	20031226
	060305				
				BA, BB, BG, BR, BY,	BZ, CA, CH, CN,
				DZ, EC, EE, ES, FI,	
	GM. HR. HU.	ID. II.	IN IS.	JP, KE, KG, KP, KR,	KZ. LC. LK. LR.
				MK, MN, MW, MX, MZ.	
				SG, SK, SL, TJ, TM,	
	UA, UG, US,				111, 111, 10,
nu.				SD, SL, SZ, TZ, UG,	7M 7W NW N9
KW:				AT, BE, BG, CH, CY,	
				IT, LU, MC, NL, PT,	
	TR, BF, BJ,	CF, CG,	CI, CM,	GA, GN, GQ, GW, ML,	MR, NE, SN, TD,
TG					
US 2004	171075	A1	20040902	US 2003-746545	20031224
US 2004	176395	Al	20040909	US 2003-746607	20031224
CA 2511	840	Al	20040722	US 2003-746545 US 2003-746607 CA 2003-2511840 AU 2003-303639 EP 2003-814980 GB GB IT LI LU	20031226
AU 2003	303639	A1	20040729	AU 2003-303639	20031226
EP 1590	344	A2	20051102	EP 2003-814980	20031226
R:					
	IE, SI, LT,	LV, FI,	, RO, MK,	CY, AL, TR, BG, CZ,	EE, HU, SK
BR 2003	017863	A	20051206	BR 2003-17863	20031226
CN 1756	849	A	20060405	CN 2003-80110049	20031226
CN 1791	596	A	20060621	BR 2003-17863 CN 2003-80110049 CN 2003-80110048 JP 2005-508623 US 2002-437304P	20031226
JP 2006	519765	T	20060831	JP 2005-508623	20031226
PRIORITY APP	LN. INFO.:			US 2002-437304P	P 20021231
				US 2002-437403P	P 20021231
				US 2002-437415P	p 20021231
				03 2002-43/4138	
				US 2002-437487P	P 20021231
				US 2003-463804P	P 20030418
				US 2003-746545	A 20031224
				US 2003-746607	A 20031224
				WO 2003-US41425	W 20031226

OTHER SOURCE(S): MARPAT 141:140459

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

726192-45-6 HCAPLUS Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(4-methyl-3-(14-phenyl-2-pyrimidinyl)aminojphenyl]- (9C1) (CA INDEX NAME)

726192-60-5 HCAPLUS
Benzamide, 4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-methyl-3-(2-pyrimidinylamino)phenyl]- (9CI) (CA INDEX NAME)

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-00-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl](9C1) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612527-99-8P 612528-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfamides as anti-cancer agents)
612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 Jun 2004
ACCESSION NUMBER: 2004:491593 HCAPLUS
TITLE: 2004:491593 HCAPLUS
141:54348
Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as inhibitors of protein tyrosine phosphatase lB
INVENTOR(5): Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin
ASTATAZENECA AB, Swed.; Astrazeneca UK Limited
PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: LANGUAGE: Patent
LANGUAGE: PATENT INFORMATION: 1
English
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND DATE		DATE
WO 2004050646	A1 20040617	WO 2003-GB5120	20031126
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BY, BZ,	CA, CH, CN
CO, CR, CU,	CZ, DE, DK, DM,	DZ, EC, EE, EG, ES, FI,	GB, GD, GE
GH, GM, HR,	HU, ID, IL, IN,	IS, JP, KE, KG, KP, KR,	KZ, LC, LK
LR, LS, LT,	LU, LV, MA, MD,	MG, MK, MN, MW, MX, MZ,	NI, NO, NZ
OM, PG, PH,	PL, PT, RO, RU,	SC, SD, SE, SG, SK, SL,	SY, TJ, TM
TN, TR, TT,	TZ, UA, UG, US,	UZ, VC, VN, YU, ZA, ZM,	ZW
		SD, SL, SZ, TZ, UG, ZM,	
		AT, BE, BG, CH, CY, CZ,	
		IT, LU, MC, NL, PT, RO,	
TR, BF, BJ,	CF, CG, CI, CM,	GA, GN, GQ, GW, ML, MR,	NE, SN, TD

AU 2003302626 PRIORITY APPLN. INFO.: 20040623 20031126 A 20021129 WO 2003-GB5120 W 20031126

OTHER SOURCE(S): MARPAT 141:54348

Title compds. I [wherein Rl = H, (halogeno)alkyl, (hydroxy)alkoxy, alkylamino, etc.; R2 = H, (halogeno)alkyl, halogeno, alkoxy; R3 = alkylamido or (un)substituted alkyl; R4 = H, alkyl, (hetero)aryl; R5 = H or alkyl; and pharmaceutically acceptable salts thereof] were prepared as inhibitors of protein tyrosine phosphatase 18 (PTB18). For example, 5-[4-(accamidomethyl)-2-methoxyphenyl]-1,2,5-thiadiazolidin-1-one 1,1-dioxide (II) was given in multi-step synthesis starting from

705256-54-8 HCAPLUS
Benzeneacetonitrile, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(9C1) (CA INDEX NAME)

705256-55-9 MCAPLUS
Acetamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methoxyphenyl]methyl]- [9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 705256-72-0 HCAPLUS (Continued)

Benzenepentananide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Ph- (CH₂)₄-C-NH-CH₂

705256-78-6 HCAPLUS Acetamide, N-[(4-(3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-82-2 HCAPLUS Acetamide, N.-(2-{4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]- (9CI) (CA INDEX NAMZ)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

705256-61-7 HCAPLUS Butanamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)- (9CI) (CA INDEX NAME)

705256-67-3 HCAPLUS Benzenepropanaide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-methyl- (9CI) (CA INDEX NAMZ)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN ED Entered STN: 21 May 2004 ACCESSION NUMBER: 2004:412929 HCAPLUS DOCUMENT NUMBER: 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 | 140:423678 |

ones as inhibitors of protein tyrosine phosphatase 1B Birch, Alam Martin; Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 89 pp. CODEN: PIXXD2 Patent English

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DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. | NO 2004041799 | Al 20040521 | WO 2003-G64721 | Z0031103 | W1 RE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CC, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GC, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LK, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MZ, NI, NO, NZ, CM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW; BW, GH, GM, KZ, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,

AU 2003278392 PRIORITY APPLN. INFO.: W 20031103

OTHER SOURCE(S):

MARPAT 140:423678

AB The title compds. (I) or pharmaceutically acceptable salts thereof [Rl = H, halo, Cl-6 alkyl, Cl-6 alkoxy, Cl-6 alkylthio, halo-Cl-6 alkyl, halo-Cl-6 alkoxy, halo-Cl-6 alkoxy, dihydroxy-Cl-6 alkoxy, dihydroxy-Cl-6

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(preparation of phenylthiadiazolidinones as inhibitors of protein

phosphatase 1B (PTP1B) for treatment of diabetes mellitus) 692764-76-4 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) alkoxy, C1-6 alkoxy-C1-6 alkoxy, aryloxy, aryl-C1-6 alkoxy, aryloxy-C1-6 alkoxy, aryloxy-C1-6 alkoxy, heteroaryloxy, heteroaryloxy-C1-6 alkoxy, C1-6 alkoxy, aryl-C1-6 alkoxy, C1-6 alkoxy, C1

they are attached form a 5-7 membered carbocyclic or heterocyclic ring:

and R4 are selected such that (i) R3 = hydrogen, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio or halo and R4 = aryl, biaryl, heteroaryl, C2-6 alkynyl, C3-7 cycloalkyl, arylcarbonyl, heteroarylacyloachonyl, aryl-c2-6 alkynyl, aryl-c2-6 alkynyl or heteroaryl-c2-6 alkenyl; or (ii) R4 = H, C1-6 alkyl, C1-6 alkynyl, C2-6 alkynyl, aryl-c2-6 alkenyl, aryl-c2-6 alkenyl, aryl-c2-6 alkenyl, aryl-c2-6 alkenyl, aryl-c2-6

alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6

phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
692765-08-5 HCAPIUS
[1,1'-Biphenyl]-4-carboxylic acid, 3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

692765-17-6 HCAPLUS [1,1'-Biphenyl]-3-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'-methoxy- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692764-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3'-nitro[1,1'-biphenyl]-4-yl)-, (9CI) (CA INDEX NAME)

1,2,5-Thiadiazolidin-3-one, 5-(3',5'-dichloro[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-79-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

692764-80-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin 692764-83-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-3-yl)-,1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

692764-84-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4'-(methylthio)[1,1'-biphenyl]-3-yl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

692764-85-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, S-(4'-methyl{1,1'-biphenyl}-3-yl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

692764-86-6 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-(2'-methyl{1,1'-biphenyl}-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-81-1 HCAPLUS Acetamide, N-[4'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}{1,1'-biphenyl}-3-yl}- (9CI) (CA INDEX NAME)

692764-82-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692764-87-7 HCAPLUS Acetamide, N-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)(1,1'-biphenyl]-3-yl]- (9CI) (CA INDEX NAME)

692764-88-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[3-(2-benzofuranyl)phenyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

692764-89-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-.
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-90-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[3-(5-oxezolyl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAEX)

RN 692764-91-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-cyclohexylphenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

RN 692764-92-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-benzoylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-96-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, S-(4,4'-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-97-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-4'-phenoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-98-0 HCAPLUS CN [1,1"-Biphenyl]-3-carbonitrile, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9C1) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-93-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-4-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-94-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-95-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-fluoro-4-methoxy(1,1'-biphenyl)-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-99-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-nitro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-00-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{3',4-dimethoxy[1,1'-biphenyl]-3-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-01-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-hydroxy-4-methoxy[1,1'-bipheny1]-3-y1)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-02-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4,4'-trimethoxy(1,1'-biphenyl)-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-04-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[1,3-benzodioxol-5-yl]-2-methoxyphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-09-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1E)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-10-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-{2-naphthalenyl}phenyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(hydroxymethyl)-4-methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-05-2 HCAPLUS

Acetamide, N-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-bjhenyl]-3-yl]- (9CT) (CA INDEX NAME)

RN 692765-06-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-07-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-12-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(methoxymethy1)[1,1'-bipheny1]-3-y1)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-13-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl)-,1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-14-3 HCAPLUS CN 1,2,5-Thiadlazolidin-3-one, 5-[4-methoxy-4'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

MeO O-CH₂-Ph

RN 692765-15-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1Z)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-16-5 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 5-[4'-[(1,1-dimethylethoxy)methyl]-4methoxy[1,1'-5:phenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-22-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-difluoro-4-methoxy[1,1'-biphenyl]-3yl)-,1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-23-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5'-fluoro-2',4-dimethoxy[1,1'-biphenyl]-3-yl)-,1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-24-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1':3',1''-terphenyl]-3-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-19-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-20-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-21-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

RN 692765-25-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-26-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{4-methoxy-4'-(methylthio)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4'-(1,1-dimethylethyl)-4-methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO Bu-t

RN 692765-28-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy{1,1':4',1''-terphenyl}-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

H O Pr

RN 692765-29-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro-4'-fluoro-4-methoxy{1,1'-biphenyl|-3-y|1)-,1,1-dioxide (9CI) (CA INDEX NAME)

H O C1

RN 692765-30-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1':4',1''-terphenyl]-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO CH=CH2

RN 692765-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-furany1)-2-methoxypheny1]-,
1,1-dioxide (SCI) (CA INDEX NAME)

NH NH

RN 692765-35-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-benzo(b)thien-2-yl-2-methoxyphenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

OMe NH

RN 692765-36-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[2-benzofuranyl]-2-methoxyphenyl]-, 1.1-dioxide (9C1) (CA INDEX NAME)

OME ONE N

RN 692765-37-0 HCAPLUS .
CN 1,2,5-Thiadiazolidin-3-one, 5-{4'-acetyl-4-methoxy{1,1'-biphenyl}-3-yl}-,

14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO Ph

RN 692765-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, S-[4-methoxy-3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Meo CF

RN 692765-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-{(lE)-2-(4-chlorophenyl)ethenyl]-2methoxyphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Heo C

RN 692765-33-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(4'-ethenyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued: 1,1-dioxide (9CI) (CA INDEX NAME)

H O Ac

RN 692765-38-1 HCAPLUS CN [1,1'-Biphenyl]-3-catpoxamide, 3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9C1) (CA INDEX NAME)

MEO C-NH2

RN 692765-39-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(1H-pyrazol-4-yl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

HN S N

RN 692765-40-5 HCAPLUS
CN Pyrrolidine, 1-[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1)carbonyl]- (9CI) (CA INDEX NAME)

RN 692765-41-6 HCAPLUS CN [1,1'-Siphenyl]-4-propanoic acid, 3'-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-42-7 HCAPLUS
CN Carbamic acid, [(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA
INDEX NAME)

RN 692765-43-8 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-47-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-{4-pyridinyl}phenyl}-, 1,1-doxide (9CI) (CA INDEX NAME)

RN 692765-48-3 KCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-hydroxy-4-methoxy[1,1'-biphenyl}-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-49-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(1H-indol-6-yl)-2-methoxyphenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-44-9 HCAPLUS CN [1,1"-Biphenyl]-4-carboxamide, N-cyclohexyl-3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-45-0 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(3'-amino-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 692765-46-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4'-(dimethylamino)-4-methoxy{1,1'-biphenyl}-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-50-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(2-thienyl)phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2-methoxy-5-(phenylethynyl)phenyl]-,
1,1-dioxide (8CI) (CA INDEX NAME)

RN 692765-52-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(3-phenyl-1-propynyl)phenyl]-,
1,1-dioxide (951) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 692765-53-0 HCAPLUS 1,2,5-Thiadiezolidin-3-one, 5-(5-ethynyl-2-methoxyphenyl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-54-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methyl{1,1'-biphenyl}-3-yl}-1,1-dioxide (9CI) (CA INDEX NAME)

692765-55-2 HCAPLUS
Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-3-yl]ethoxy[-6-hydroxy-(9CI) (CA INDEX NAME)

692765-56-3 HCAPLUS
Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-3-y1]ethoxy[-,6-hydroxy-,methyl ester (9CI) (CA

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-60-9 HCAPLUS
Benzoic acid, 2-{2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-4-y1)ethoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

692765-61-0 HCAPLUS
Benzoic acid, 2-[2-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-4-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA

692765-62-1 KCAPLUS
Benzoic acid, 2-(3-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy(1,1'-bipheny1|-3-y1]propoxy1-6-hydroxy-(9C1) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN INDEX NAME) (Continued)

692765-57-4 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]methoxy]-6-hydroxy-, methyl ester [9CI] (CA
INDEX NAME)

692765-58-5 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]methoxy[-6-hydroxy- [9CI] (CA INDEX NAME)

692765-59-6 HCAPLUS
Benzoic acid, 2-[{3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-4'-methoxy{1,1'-biphenyl}-4-y1]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692765-63-2 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl}-3-yl)propoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-64-3 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-4-y1]propoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

692765-65-4 RCAPLUS
Benzoic acid, 2-[3-[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-66-5 HCAPLUS
Benzoic acid, 2-[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-3-y1]methoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

692765-67-6 HCAPLUS
{1,1'-Biphenyl]-3-carboxamide,
{1,1-dioxido-4-oxo-1,2,5-thiadiarolidin2-yl)-4'-methoxy-N-{2-phenoxyethyl}- (9CI) (CA INDEX NAME)

RN 692765-68-7 HCAPLUS
CN Benzoic acid,
2-[2-[[[]3'-[],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid,
2-[[6-[[[3]-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'metchoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]hexyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

- (CH2)6-NH

RN 692765-72-3 HCAPLUS
CN Benzoic acid,
2-[2-[[[3]*-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

692765-73-4 HCAPLUS

RN 692765-73-4 HCAPLUS

CN Benzoic acid,
2-[3-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl|carbonyl|amino|propoxy|-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

RN 692765-74-5 HCAPLUS CN Benzoic acid, 2-{[5-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-692765-74-5 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-69-8 HCAPLUS
CN Benzoic acid,
2-[3-[{[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-4'methoxy[1,1'-biphenyl}-3-yl]carbonyl]amino]propoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

RN 692765-70-1 HCAPLUS
CN Benzole acid,
[5-[15-[13'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy(1,1'-bipheny1]-3-y1)carbony1)amino]penty1]oxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX MAME)

692765-71-2 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) methoxy[1,1'-bipheny1]-4-y1[carbony1]amino[penty1]oxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

692765-79-0P 692765-80-3P 692765-84-7P
692765-85-8P 692765-86-9P 692766-02-2P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation of phenylthiadiazolidinones as inhibitors of protein

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-80-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-84-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(5-bromo-2-methoxyphenyl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

692765-85-8 HCAPLUS
Boronic acid, [3-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4-methoxyphenyl1- (9CI) (CA INDEX NAME)

692765-86-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 10 OCC 2003 ACCESSION NUMBER: 2003:796679 HCAPLUS DOCUMENT NUMBER: 139:307766

TITLE:

Preparation of substituted 1,1-dioxo-1,2,5-thiazolidine-3-ones as protein tyrosine phosphatase

INVENTOR(S):

and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabates or atherosclerosis Coppola, Gary Mark: Davies, John William: Jewell, Charles Francis, Jr.; Li, Yu-Chin: Mareing, James Richard; Sperbeck, Donald Mark: Stams, Travis Mathew: Topiol, Sidney Wolf; Vlattas, Isidoros Novartis A.-G., Switz:, Novartis Pharma G.m.b.H. PCT Int. Appl., 148 pp. CODEN: PIXXD2
Patent
English

WO 2003-EP3466

W 20030402

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PAT	ENT :	KIND		DATE		APPLICATION NO.						DATE						
	WO	WO 2003082841				A1		20031009		WO 2003-EP3466						20030402			
		W:	AE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG;	BR,	ΒY,	BZ,	CA,	CH,	CN,	
			co,	CR,	Cυ,	cz,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
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	US 2004023974				A1	A1 20040205				US 2003-405728						20030402			
	EP 1492780				A1	A1 20050105				2003-720412						20030402			
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										CY,	AL,	TR,	BG,	cz,	EE,	ΗU,	SK		
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	NO	2004	0047	45		A		2004	1214		NO 2	2004-	4745			2	0041	102	
PR	IORIT	APP	LN.	INFO	. :						US 2	2002-	3697	79P		P 2	0020	403	
											US 2	2002-	3699	30P		P 2	0020	403	

OTHER SOURCE(S): MARPAT 139:307766 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) dioxaborolan-2-yl)phenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692766-02-2 KCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{5-iodo-2-methoxyphenyl}-, 1,1-dioxide CN (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Substituted thiazolidinetriones I [L1 = L2 = single bond; Q1 = single bond, H, (un)substituted alkyl, cycloalkyl, or aminocarbonyl, carboxy, RIOC(:O), RIOC(:O), RIOS(:O)q; Q2 = O, S, R3N; R, R2 = (un)substituted alkyl, alkynyl, heteroalkyl, aryl, heteroarkyl, aralkyl, alkoxy, aralkoxy, or aralkylthio, amino, halogen, nitro, carboxy, trifluoromethyl, etc.; R1 = (un)substituted alkyl, alkoxy, aralkoxy, aralkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, aralkylthio; R3 = H, HO, alkyl; R1O = (un)substituted alkyl, alkoxycarbonyl, aryl, heteroaryl, aralkyl, R1C = (un)substituted alkyl, alkoxycarbonyl, acyl, aryloxycarbonyl, heteroaryloxycarbonyl, carbamoyl, or sulfonyl; X, T = CH, N, O, S, R14N; Z = (un)substituted alkyl, alkoxyalkyl, alkylthioalkyl, alkylaminoalkyl; Z1, Z2, Z3 = CH, N, N(:O), CR1, CR2; R1 and R2 can form an (un)substituted 5 -, or 6-membered aromatic or heteroarom. ring; R1 and L1 can form an (un)substituted 5 -, or

or
7-membered ring interrupted by nitrogen, oxygen or sulfur atoms] such as
II are prepared as inhibitors of protein tyrosine phosphatase 1b and

protein tyrosine phosphatase for overcoming insulin resistance and modulating glucose levels in the treatment or prevention of metabo-diseases, such as diabetes, or atherosclerosis. II is prepared by

treatment
of Et bromoacetate with 1-naphthalenemethanamine, N-sulfamoylation with
sulfamoyl chloride, and base-mediated cyclocondensation. No biol. data

Provided.
612330-89-9 612530-90-2P 612530-92-4P 612330-93-5P 612530-93-6P 612530-99-1P 612530-98-6P 612530-98-9P 612530-98-0P 612531-095-7P 612531-00-1P 612531-05-2P 612531-00-9P 612531-00-9P 612531-00-9P 612531-03-9P 612531-19-2P 612531-19-2P 612531-19-3P 612531-19-3P 612531-19-5P 612531-19-5P 612531-19-5P 612531-19-5P 612531-19-5P 612531-60-9P 612531-79-9P 612531-79-9P 612531-79-0P 612531-79-0P 612531-79-0P 612531-79-0P 612531-79-0P 612531-79-0P 612531-79-0P

ANSWER 15 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612531-80-3P 612534-94-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate; prepn. of thiazolidinetriones as protein tyrosine
phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to
mitigate insulin resistance in the treatment of diabetes or
atherosclerosis)
612530-89-9 KCAPLUS
Carbanic acid, (4-[5-((2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

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RN 612530-90-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[(2,4-dimethoxyphemyl]methyl]-5-[(1-ethyl-2methyl-1H-benzimidazol-5-yl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612530-92-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-[(4-methoxy-7-quinolinyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-93-5 HCAPLUS
CN Benroic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, [4-(methylthio)phenyl]methyl ester (9CI)
(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-94-6 HCAPLUS
CN Benzoic acid,
4-[55-[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5thiadiarolidin-2-yl]methyl]-, [4-(methylsulfonyl)phenyl]methyl ester (9CI)

(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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(Continued)

(Continued)

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612530-95-7 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 5-[[4-(bromomethyl)phenyl]methyl]-2-[(2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2Br

RN 612530-96-8 HCAPLUS
CN Acetic acid, [[[4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI)
(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A | OMe

RN 612530-99-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-iodophenyl)methyl]-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-98-0 HCAPLUS
CN Acetic acid, [[[4-[[5-(2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl[methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612531-00-7 HCAPLUS CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl], phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-01-8 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[(5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (GC INDEX NAME)

Absolute stereochemistry.

RN 612531-02-9 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[(4-methoxyphenyl)methyl)-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-2-oxo-2(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-03-0 HCAPLUS Benzenepropananide, α -amino-3-[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-N-pentyl-, (α S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-13-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl)-5-[[4-[4-(qhenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

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L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-05-2 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-10-9 HCAPLUS

EN Benzaldehyde,

4-[[5-[(2,4-dinethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612531-22-3 HCAPLUS
Carbamic acid, [[4-[[5-[(2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (SCI) (CA INDEX NAME)

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612531-23-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-2-[{2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612531-31-4 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5 thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612531-30-3 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-32-5 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-{(1,1-dimethylethoxy)carbonyl]phenyl]methyl ester (9CI) {CA INDEX NAME}

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RN 612531-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-(2,4-dinitrophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

IN 612531-35-8 HCAPLUS
IN 1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-2-[(2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612531-63-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-2-((4-methoxyphenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-64-3 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-4-{5-{(4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-36-9 HCAPLUS
CN Benzoic acid, 3-[5-[{2,4-dimethoxyphenyl}methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, methyl ester (9CI) {CA INDEX NAME}

RN 612531-61-0 HCAPLUS
CN 1H-1,4-Benzodiazepine-2,5-dione, 3-[[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-(phenylmethoxy)phenyl]methyl]-3,4-dihydro-(9CI)(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612531-65-4 HCAPLUS
CN D-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-66-5 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-4-[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-67-6 HCAPLUS
CN Carbamic acid,
[(1S)-1-[[4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yllphenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-68-7 HCAPLUS
Benzenepropanamide, a-amino-4-[5-[(4-methoxyphenyl)methyl]-1,1dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

612531-69-8 HCAPLUS L-Phenylalanyl-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612531-72-3 HCAPLUS
L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-[(4-methoxyphenyl)methyl]1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-73-4 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-[2-(1,1-dimeth)dehoxy]-2-oxethyl]phenyl]ethyl]-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

612531-70-1 HCAPLUS L-Phenylalanine, 4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-71-2 HCAPLUS L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-[{4-methoxyphenyl}methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-75-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-76-7 HCAPLUS CN 1,2,5-Thiadistolidin-3-one, 5-(3-iodopheny1)-2-([4-methoxypheny1)methy1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-77-8 HCAPLUS
L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-,phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-78-9 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl}-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI)(CA INDEX NAME)

Absolute stereochemistry.

(Continued) ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612534-94-8 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI)- (CA INDEX NAME)

Absolute stereochemistry.

612527-93-2P 612530-46-8P 612530-49-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (invention compound; preparation of thiazolidinetriones as protein sine

sine
phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to
mitigate insulin resistance in the treatment of diabetes or
atherosaclerosis)
612527-93-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-aminophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612531-79-0 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

(Continued)

Absolute stereochemistry.

612531-80-3 HCAPLUS
Benzenepropanamide, q-amino-3-[S-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (a5)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-46-8 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
ester (9CI) (CA INDEX NAME)

612530-49-1 HCAPLUS
Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, methyl ester (9CI) (CA INDEX NAME)

612527-84-1P 612527-85-2P 612527-86-3P 612527-91-4P 612527-80-5P 612527-99-6P 612527-93-99-6P 612527-93-99-6P 612527-93-99-6P 612527-93-1P 612527-93-99-6P 612528-00-4P 612528-01-5P 612528-03-99-3P 612528-01-6P 612528-03-4P 612528-03-4P 612528-03-4P 612528-03-4P 612528-03-4P 612528-03-4P 612528-03-4P 612528-13-99-3P 612528-13-99-3P 612528-13-99-3P 612528-13-99 6125289

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ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612530-08-2P 612530-09-3P 612530-10-6P
612530-11-7P 612530-12-8P 612530-13-9P
612530-16-2P 612530-12-8P 612530-18-4P
612530-19-5P 612530-20-8P 612530-21-9P
612530-22-0P 612530-23-1P 612530-28-6P
612530-22-7P 612530-31-3P 612530-28-6P
612530-22-7P 612530-31-3P 612530-28-6P
612530-32-P 612530-31-3P 612530-31-1P
612530-35-5P 612530-31-3P 612530-37-7P
612530-38-8P 612530-31-9P 612530-31-P
612530-41-3P 612530-42-4P 612530-47-9P
612530-44-9P 612530-45-7P 612530-47-9P
612530-48-0P 612530-65-7P 612530-47-9P
612530-48-0P 612530-50-4P 612530-47-9P
612530-48-0P 612530-47-4P 612530-47-9P
612530-48-0P 612530-47-4P 612530-47-9P
612530-48-0P 612530-47-4P 612530-47-9P
612530-48-0P 612530-47-4P
612530-48-0P 612530-47-

612527-85-2 HCAPLUS
Acetamide, N-[[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}pheny1}methy1]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN __(Continued)

612527-86-3 HCAPLUS Carbamic acid, [[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl}-, l,1-dimethylethyl ester (9CI) (CA (CA INDEX NAME)

612527-87-4 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612527-88-5 HCAPLUS Acetamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN y1)methy1]pheny1]methy1]- (9CI) (CA INDEX NAME)

612527-89-6 HCAPLUS
Carbamic acid, [(4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y)]methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (9Cl) (CA INDEX NAME)

612527-90-9 HCAPLUS
Benzenepropanamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]nethyl]- [9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-91-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(3-iodophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-92-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-nitrophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)

RN 612527-98-7 HCAPLUS
CN Urea,
N-[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-N'propyl- (9CI) (CA INDEX NAME)

612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-94-3 HCAPLUS
Acetamide, N-[3-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl)- (9C1) (CA INDEX NAME)

612527-96-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{4-aminophenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-97-6 HCAPLUS
Butanamide, N-[3-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-00-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl](9CI) (CA_INDEX_NAME)

612528-01-5 HCAPLUS
Benzoic acid, 2-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-(9CI) (CA INDEX NAME)

612528-02-6 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methylphenyl)methyl]-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612528-07-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-08-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-amino-2-bromophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-11-7 HCAPLUS
CN Methanesulfonamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612528-12-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methylphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-09-3 HCAPLUS
CN Acetamide, N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 612528-10-6 HCAPLUS
CN Methanesulfonamide, N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612528-13-9 HCAPLUS

N Benzeneacetic acid, α-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}- (9CI) (CA INDEX NAME)

RN 612528-14-0 HCAPLUS
CN Benzeneacetamide, α-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-15-1 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzeneacetamide, a-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-16-2 HCAPLUS Benzeneacetamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-y1)methyl]-N-propyl- α -[(trifluoroacety1)amino]- (9CI) (CA INDEX NAME)

RN 612528-17-3 HCAPLUS
CN Benzeneacetamide,
4-[(1,1-d(\oxido-4-0x-1,2,5-thiadiazolidin-2-yl)methyl]u-{{methylsulfonyl)amino}-N-propyl- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-20-8 HCAPLUS Benzenepropanamide, α -amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]-N-propy1- (9CI) (CA INDEX NAME)

612528-21-9 HCAPLUS .
Phenylalanine, N-acetyl-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

612528-18-4 HCAPLUS Benzenepropanamide, α -(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-propyl- (9CI) (CA INDEX NAME)

.612528-19-5 HCAPLUS
Propanedioic acid, {acetylamino}[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX

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612528-22-0 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-q-phenyl-, 1,1-dioxide (9C1) (CA INDEX NAME)

612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-25-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3,4-dimethoxyphenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-26-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(2-chlorophenyl)ethyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-27-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(4-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-32-2 HCAPLUS CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -(phenylmethyl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-33-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-34-4 HCAPLUS

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-28-6 HCAPLUS CN Acetamide N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)ethyl]phenyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

RN 612528-29-7 HCAPLUS
CN Butanamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)-1-naphthalenyl]methyl]-,
1,1-dicxide (9CI) (CA INDEX NAME)

RN 612528-35-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-36-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-methyl]-1-(3-methylbutyl)-1H-benzimidazol-5-yl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-37-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxy-7-quinolinyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-38-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(2-methylpropoxy],7-quinolinyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-39-9 HCAPLUS Glycine, N-[2-(butylamino)-2-oxo-1-phenylethyl)-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-40-2 HCAPLUS
Glycine, N-[2-(butylamino)-1-(4-ethylphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-42-4 HCAPLUS Glycine, N-[2-(burylamino)-1-(4-methoxyphenyl)-2-oxoethyl]-N-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]- {9CI} (CA INDEX

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612528-41-3 HCAPLUS
Glycine, N-[2-(butylamino)-2-oxo-1-(3-phenoxyphenyl)ethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (GA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-43-5 HCAPLUS Glycine, N-[1-(2-bromophenyl)-2-{butylamino}-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

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612528-44-6 HCAPLUS Glycine, N-[2-(butylamino)-1-(2-naphthalenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612526-45-7 HCAPLUS Glycine, N-[2-(butylamino)-1-(4-chlorophenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

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ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN NAME) (Continued)

RN 612528-48-0 HCAPLUS
CN Glycine,
N-[1=[(burylamino)carbonyl]-3-phenylpropyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-49-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(methylsulfonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-46-8 HCAPLUS
Glycine, N-[2-(butylamino)-2-oxo-1-[3-(phenylmethoxy)phenyl]ethyl]-N-[4[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA
INDEX NAME)

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RN 612528-47-9 HCAPLUS
CN Glycine,
N-[(ZE)-1-[(butylamino)carbonyl]-3-phenyl-2-propenyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612528-50-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(3-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

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612528-51-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
(4-butylphenyl)methyl ester (9CI) (CA INDEX NAME)

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612528-53-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[2-(2-phenylethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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- 612528-52-6 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 [4-(hydroxymethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

- 612528-54-8 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
 {1,1'-biphenyl}-2-ylmethyl ester (9CI) (CA INDEX NAME)

- 612528-55-9 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 [4-(difluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)

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RN 612528-56-0 HCAPLUS
CN 2-Thiopheneacetic acid,
5-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]oxy]methyl]-α,α-difluoro-(9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612528-59-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{{4-[(3-methylbucyl)thio)methyllphenyl}meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me2CH-CH2-CH2-S-CH2

612528-60-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-ethylbutyl ester (9CI) (CA INDEX NAME)

612528-61-7 HCAPLUS
Benzoic acid, 4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclobutylmethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-57-1 HCAPLUS
Acetic acid, {[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

612528-58-2 HCAPLUS Acetic acid, [[(4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI) (CA IMDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-62-8 HCAPLUS
Benroic scid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl)methyl]-,
cyclopentylmethyl ester (9CI) (CA INDEX NAME)

612528-63-9 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-methylpentyl ester (9CI) (CA INDEX NAME)

612528-64-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2,4,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-65-1 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclohexylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-66-2 HCAPLUS |
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
1,2-dimethylpropyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-69-5 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2-(methylthio)ethyl ester (9CI) (CA INDEX NAME)

RN 612528-70-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-[(carboxymethyl)thio]ethyl ester (9CI) (CA INDEX NAME)

RN 612528-71-9 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(5-nitro-2-furanyl)methyl ester (9CI) (CA INDEX NAME) .

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-67-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
cyclopentyl ester (9CI) [CA INDEX NAME]

RN 612528-68-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylbutyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-72-0 HCAPLUS
Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-pytdidnylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-73-1 HCAPLUS
CN Benzole acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
[3-(kydroxymethyl)phenyl]methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

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RN 612528-74-2 HCAPLUS
Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-,
[3-(methylsulfonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

(Continued)

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L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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RN 612528-75-3 HCAPLUS
CN Benzeneacetic acid, 4-[4-[{4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]amino]butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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N 612528-76-4 HCAPLUS
N Benzeneacetic acid, 4-{3-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]benzoy1]amino]propy1]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN

(Continued)

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- RN 612528-77-5 HCAPLUS
 CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
 [5-{(dimethylamino)methyl}-2-furanyl}methyl ester (9CI) (CA INDEX NAME)
- N-CH2-NMe2
- RN 612528-78-6 HCAPLUS

 L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

RN 612528-79-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(1H-indol-5-ylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-80-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3,4,5-trimethoxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-82-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[4-(phenylmethyl)-1piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (SCI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-85-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-86-6 HCAPLUS 1,2;5-Thiadiazolidin-3-one, S-[[4-(4-methyl-1-oxopentyl)phenyl]methyl]-, 1,1-dioxide (9c1) (CA INDEX NAME)

RN 612528-87-7 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 5-[[3-(2-fluorophenoxy)phenyl]methyl]-,
1,1-dioxide [9C1] (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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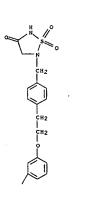
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RN 612528-83-3 HCAPLUS
CN Benzeneacetic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

RN 612528-84-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-benzoylphenyl)methyl}-, 1,1-dioxide
(9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612528-88-8 HCAPLUS
CN Benzoic acid, 3-[2-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]ethoxy]- (9CI) (CA INDEX NAME)



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RN 612528-89-9 HCAPLUS CN 2(IH)-Quinolinone, 6-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

CH2-CH2-CHMe2

RN 612528-97-9 HCAPLUS CN Acetamide, 2-amino-N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2y1]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

H₂N-CH₂-C-NH-CH₂

RN 612528-98-0 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
(4-carboxyphenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-00-7 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3nitro- (9CI) (CA INDEX NAME)

02N CH2

RN 612529-01-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

HO-CH2

RN 612529-02-9 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl-, methyl ester (9C1) (CA INDEX MAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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N 612528-99-1 HCAPLUS N 1,2,5-Thiadiazolidin-3-one, 5-{{3-phenoxyphenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

14 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

H₂N C-OMe

RN 612529-03-0 HCAPLUS CN 1,2,5-Thiadlazolidin-3-one, 5-[(4-hydroxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

H N S

RN 612529-04-1 HCAPLUS
CN Benzoic acid, 2-{(l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-5-nitro-(9CI) (CA INDEX NAME)

HO₂C HO₂C

RN 612529-05-2 HCAPLUS
CN Benzoic acid, 5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]- (9Cl) (CA INDEX NAME)

HO2C HO2C

RN 612529-06-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-chloro-3-methoxy-5-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612529-10-9 HCAPLUS CN 1,2,5-Thladdazolidin-3-one, 5-(3-phenylpropyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{{4-butoxyphenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-12-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-(trifluoromethyl)phenyl)methyl)-,
1,1-dioxide (SCI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-07-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-08-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methyl-2-nitrophenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-09-6 HCAPLUS

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-13-2 HCAPLUS
CN Benzoic acid, 3-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

RN 612529-14-3 HCAPLUS CN Benzenebutanoic acid, 5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)methyl]- (9CI) (CA INDEX NAME)

RN 612529-15-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{{2-methyl-3-nitrophenyl}methyl}-,
1,1-dioxide {9CI} (CA INDEX NAME)

1.4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[{4-methyl-3-nitrophenyl}methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-17-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(5-methyl-2-nitrophenyl)methyl}-,
1,1-dloxide (921) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

RN 612529-22-3 HCAPLUS
CN Acetic acid, [[2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]anino]oxo- (9CI) (CA INDEX NAME)

RN 612529-23-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(3-hydroxyphenyl)methyl}-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612529-24-5 HCAPLUS
CN Benzoic acid, 2-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]- {9CI} (CA INDEX NAME}

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 612529-18-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-aminophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

RN 612529-19-8 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[4-[4,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612529-20-1 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612529-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[1,4-phenylenebis(methylene)]bis-,
1,1,1'-tetraoxide (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-26-7 HCAPLUS CN 1,2.5-Thiadiazolidin-3-one, 5-[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-27-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3-(hydroxymethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-28-9 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[[3-amino-5-(hydroxymethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-29-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-4-methylphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-30-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-3-methylphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-36-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-37-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-hydroxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-31-4 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[(3-amino-2-methylphenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-32-5 HCAPLUS
.1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-5-methylphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME);

612529-33-6 HCAPLUS Acetamide, N-[(4-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-38-1 HCAPLUS 1,2.5-Thiadiazolidin-3-one, 5-[(3,5-dimethylphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-39-2 HCAPLUS
L-Phenylalanine, N-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl}methyl]-, ethyl ester (9CI) (CA INDEX NAME)

612529-40-5 HCAPLUS L-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

612529-41-6 HCAPLUS
Benzoic acid, 2-amino-5-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-42-7 HCAPLUS
CN Benzoic acid,
2-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-43-8 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 5-[[2-(phenylmethyl)phenyl]methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612529-44-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2,4-bis(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

(Continued)

RN 612529-45-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,4,6-trifluorophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-46-1 HCAPLUS
CN 1,2,5-Thiadiezolidin-3-one, 5-[(2-bromophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

RN 612529-47-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[[1,1'-biphenyl]-2,2'diylbis(methylene)]bis-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

RN 612529-48-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[ethylamino]methyl]phenyl]methyl]-,
1,1-dioxide (901) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued Benzoic acid, 2-(acetylamino)-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl)- (9Cl) (CA INDEX NAME)

RN 612529-50-7 HCAPLUS
CN Benzoic acid, 2-amino-4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl|-, ethyl ester (9CI) (CA INDEX NAME)

RN 612529-51-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-[((2-phenylethyl)amino]methyl]phenyl]met hyl), 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-49-4 HCAPLUS

Ph-CH2-CH2-NH-CH2

RN 612529-52-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-{{diethylamino}methyl}phenyl}methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-53-0 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-57-4 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(3-methylbutyl)- (901) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-54-1 HCAPLUS
CN Benzamide, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 612529-56-3 HCAPLUS
CN Benzamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[2-[3-(trifluoromethyl)phenyl)ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612529-58-5 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-a-(phenylmethyl)-,
1,1-dioxide, (ds)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-59-6 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-α-(phenylmethyl)-,
1,1-dioxide, (αR)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-60-9 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-61-0 HCAPLUS
Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenoxy]- (9CI) (CA INDEX NAME)

612529-62-1 HCAPLUS
Benzolc acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylpropyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-65-4 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-y1)methyl}-,
[4-{carboxymethoxylphenyl]methyl ester (9C1) (CA INDEX NAME)

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L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-63-2 HCAPLUS
Benzoic acid, 2-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}-, 2-methy1propy1 ester (9CI) (CA INDEX NAME)

612529-64-3 HCAPLUS
Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenoxy]-, methyl ester [9CI] (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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(Continued)

612529-67-6 HCAPLUS
Benzoic acid, 4-[2-[[[4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

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$$\Diamond$$

RN 612529-68-7 HCAPLUS
CN Acetic acid, [4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenoxy]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-69-8 HCAPLUS
Acetic acid, [4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]phenoxy}-, phenylmethyl ester (9CI) (CA INDEX NAME)

612529-70-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-75-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-76-7 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one, 5-[(4-ethoxyphenyl)methyl]-, 1,1-dioxide
(9CI)

(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-73-4 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

612529-74-5 HCAPLUS.

Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-3-nitro-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-77-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{[3-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-78-9 HCAPLUS
Benzeneacetic acid, 4-{[[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}benzoyl]oxy]methyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612529-79-0 HCAPLUS
CN Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-phenylethyl etter (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE

RN 612529-82-5 HCAPLUS Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, [4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl}methyl ester (9C1) (CA INDEX NAME)

RN 612529-83-6 HCAPLUS
CN Benzoic caid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-80-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(phenylamino)ethyl ester (9CI) (CA INDEX NAME)

RN 612529-01-4 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
2-(3-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

IA ANSWER 15 OF 33 HCARLUS COPYRIGHT 2006 ACS on STN (Continu

RN 612529-84-7 HCAPLUS
CN Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
3-methoxy-2,2-dimethyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

RN 612529-85-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2,2,4-trimethylpentyl ester {9CI} (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-86-9 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
3-(dimethylamino)-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

612529-87-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
[(3a, 4,5,8,6a5)-5-(benzoyloxy)hexahydro-2-oxo-2H-cyclopenta[b]furan-4yl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-91-6 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
(3-chloro-4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

612529-93-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl)-,
6-ethoxy-6-oxohexyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-90-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methýl]-,
(3-methyl-4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

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612529-94-9 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(3-chlorophenyl)ethyl ester (9Cl) (CA INDEX NAME)

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L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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612529-95-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(3-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)

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612529-96-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-98-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(phenylmethyl)amino]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-99-4 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,(4-methyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-(3-(trifluoromethyl)phenyl)ethyl ester (9CI) (CA INDEX NAME)

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612529-97-2 HCAPLUS
D-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

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612530-01-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(methoxycarbonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-02-6 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-cyclohexyl-2-methylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-04-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

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L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-03-7 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-phenoxypropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Cont

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RN 612530-05-9 HCAPLUS
CN Benzolc acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
[3-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

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CF3

RN 612530-06-0 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(4-czeboxyphenyl)athyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (C

(Continued)

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DACE 2-1

RN 612530-08-2 HCAPLUS
CN Benzoic acid, 3-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

i-BuNH-CH2

RN 612530-10-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-1-one,
5-[[4-[[(2,2-dimethyl]propyl)amino]methyl]pheny
l]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) .

Me3C-CH2-NH-CH2

RN 612530-11-7 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
1-naphthalenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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CO2H

RN 612530-09-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(2-methylpropyl)amino]methyl]phenyl]me
thyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

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RN 612530-12-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-13-9 HCAPLUS
CN Benzeneacetic acid, 4-[2-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]amino]ethyl]- [9CI] (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2

RN 612530-17-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)-,
3-[(carboxymethyl)amino]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-18-4 HCAPLUS

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N

CH2

NH

CH2

CH2

CH2

RN 612530-16-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
(3-nitrophenyl)methyl ester {9CI} (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- [9CI] (CA INDEX NAME)

RN 612530-19-5 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
[1,1'-biphenyl]-4-ylmethyl ester (9CI) (CA INDEX NAME)

RN 612530-20-8 HCAPLUS

- L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
 [4-(acetylamino)phenyl]methyl ester (9CI) (CA INDEX NAME)

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- RN 612530-21-9 HCAPLUS
 CN Benzole acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]-,
 (2-(phenylmethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

- L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (2-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)
 - PAGE 1-A

 O

 N

 CH2

 CH2

 Me
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- RN 612530-25-3 HCAPLUS

 Senzeneacetic acid. 3-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl[oxy]methyl]- (9CI) (CA INDEX NAM2)

- L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
- Ph-CH2
- RN 612530-22-0 HCAPLUS
 CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
 (2-methylphenyl)methyl ester (9CI) (CA INDEX NAME)
- RN 612530-23-1 HCAPLUS
 CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
- L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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CH2-CO2H

RN 612530-26-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

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RN 612530-27-5 HCAPLUS

Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

[4-fluoro-2-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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_ OMe

RN 612530-29-7 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI)
(CA INDEX NAME)

RN 612530-30-0 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
(5-methyl-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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RN 612530-28-6 HCAPLUS
CN Benzoic acid,
4-[55-[42.4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)phenyl]methyl ester (9CI) (CA INDEX NAME)

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RN 612530-31-1 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-methylphenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-32-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
3-((carboxymethyl)methylamino]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-33-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, phenyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-37-7 HCAPLUS
CN 1-Piperazineacetic acid, 4-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9C1) (CA INDEX NAME)

RN 612530-38-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
2-naphthalenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-34-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[5-[((2-methyl)propyl)amino]carbonyl}-2-thienyl]methyl ester (9CI) (CA
INDEX NAME)

RN 612530-35-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenylmethyl ester (9CI) (CA INDEX NAME)

RN 612530-36-6 HCAPLUS
CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N,N-bis(2-methylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-39-9 HCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[[{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y-l)methyl]benzoyl]oxy]methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-40-2 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(aminocarbonyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-41-3 HCAPLUS
CN Piperazine, 1-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-42-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(1-oxo-3-phenylpropyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

612530-43-5 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl}methyl}-,
[5-[[qhenylmethyl]amino]carbonyl]-2-thienyl]methyl ester (\$CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-48-0 HCAPLUS .
1,2,5-Thiadiazolidin-3-one, 5-[4-(aminomethyl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-50-4 HCAPLUS
CN Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-(9CI) (CA INDEX NAME)

612530-51-5 HCAPLUS
1,2,3-Thiadizolidin-3-one, 5-(2,4-dimethoxyphenyl)-, 1,1-dioxide, potassium salt (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-44-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-45-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{2,4-diaminophenyl}-, 1,1-dioxide (9CI) INDEX NAME)

612530-47-9 HCAPLUS Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-52-6P 612530-53-7P 612530-54-8P 612530-55-9P 612530-56-0P 612530-57-1P 612530-58-2P 612530-59-3P 612530-60-6P 612530-61-7P 612530-62-2P 612530-63-9P 612530-61-79 612530-68-4P 612530-66-2P 612530-67-3P 612530-68-4P 612530-69-5P 612530-73-3P 612530-72-0P 612530-73-1P 612530-73-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P (invention compound; preparation of thiazolidinetriones as protein

(invention compound, preparation of thiazolidinetriones as protein tyrosine

phosphatase 1b and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis)

RN 612530-52-6 HCAPLUS

CN Acetamide, 2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methylphenoxy}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

612530-53-7 HCAPLUS
1H-1,4-Benzodiazepine-2,5-dione, 3-[[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-hydroxyphenyl]methyl]-3,4-dihydro-(9CI) (CA

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)

RN 612530-54-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-55-9 HCAPLUS
CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-,
phenylmethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-56-0 HCAPLUS CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

H O HN S Ph NHAC

RN 612530-60-6 HCAPLUS
CN L-Phenylalaninamide, N-benzoyl-O-(dicarboxymethyl)-L-tyrosyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-61-7 HCAPLUS
CN Benzenepropanamide, α={([1,1'-biphenyl]-4-ylsulfonyl)amino]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 612530-57-1 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-58-2 HCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadia2olidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-59-3 HCAPLUS
CN L-Phenylalaninanide, N-acetyl-L-phenylalanyl-N-[2-[4-(carboxymethyl)phenyl]ethyl]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- [9C] (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-62-8 HCAPLUS

Renzenepropanamide, α-{{[1,1'-biphenyl]-4-ylsulfonyl}amino}-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-(4-phenylbutyl)-, (αS)-(9CI) (CA INDEN NAME)

Absolute stereochemistry.

RN 612530-63-9 HCAPLUS
CN Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-a-{{phenylsulfonyl}amino}-, {aS}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-64-0 HCAPLUS
Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)-α-((phenylsulfonyl)amino]-, (αS)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 612530-65-1 HCAPLUS
CN Benzenepropanamide,
4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(3,3-diphenylpropyl)-a-[(phenylsulfonyl)amino]-, (a\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-66-2 HCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[(4-aminophenyl)methyl]-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612527-96-5 CMF C9 H11 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612530-72-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{{1-ethyl-2-methyl-1H-benzimidazol-5-yl}methyl}-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612528-35-5 CMF C13 H16 N4 O3 S

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-67-3 HCAPLUS Benzenepropanamide, 3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- α -[(phenylsulfonyl)amino}-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-68-4 HCAPLUS L-Phenylalaninamide, etyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{phenylmethyl}-, 1,1-dioxide (9CI) {CA INDEX NAME}

612530-71-9 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM 2

612530-73-1 HCAPLUS
1,2,5-Thiediazolidin-3-one, 5-[{4-{(Z)-(3-oxo-2(3H)-benzofuranylidene)methyl}phenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

612530-74-2 HCAPLUS Ethanedione, [4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1)phenyl)phenyl- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-75-3 HCAPLUS
9,10-Anthracenedione, 2-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

612530-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide, sodium salt (9CI) INDEX NAME)

612530-78-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide, trifluoroacetate (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM (Continued)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 1

CRN 612530-45-7 CMF CB H10 N4 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612534-93-7 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 31 Jul 2002
ACCESSION NUMBER: 2002:553867 HCAPLUS
ITILE: 137:22603
Efficient Solid-Phase Synthesis of Sulfahydantoins
Trembley, Melanie: Voyer, Normand: Boujabi, Sihem,
Dewynter, Georges F.
Centre de Recherche sur la Fonction, la Structure et
l'Ingenierie des Proteines, Departement de Chimie,
Faculte des Sciences et de Genie, Universite Laval,
Quebec, OC, GLK 7P4, Can.
Journal of Combinatorial Chemistry (2002), 4(5),
429-435
CODEN: JCCHFF; ISSN: 1520-4766
American Chemical Society
Journal
LANGUAGE: Digital
CASREACT 137:232603

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB A novel solid-phase strategy allows the efficient preparation of traceless sulfahydantoins. A total of 28 derivs, with crude purity generally higher than 85%, were prepared by parallel synthesis. Through reductive alkylations, Nitsunobu reactions, and sulfamoylation reactions on oxime resin, the synthetic strategy affords sulfahydantoin derivs. selectively substituted at N2, e.g., I, N5, e.g., II, and N2, N5, e.g., III, positions, slthough yields of disubstituted compds. are lower. The mild reaction conditions involved, lead to sulfahydantoins without racemization.

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
459831-33-5P 459831-34-6P 459831-35-7P
RL: SPN (Synthetic preparation) PREP (Preparation)
(stereoselective preparation of N2,N5-disubstituted sulfahydantoins reductive alkylation of resin-bound phenylalanine with substituted benzaldehydes and subsequent sulfamoylation, Mitsunobu reaction, resin-cleavage, and cyclization)
RN 459831-33-5 MCAPUUS
CN 1,2,5-Thiadiazolidin-3-one,
5-((4-methyl)henyl)methyl)-4-(phenylmethyl)-2(2-propenyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-34-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2-butyl-5-[(4-methylphenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 459831-35-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methylphenyl)heuthyl]-4-[phenylmethyl]-2(3-phenylpropyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 283587-14-4P 459831-30-2P 459831-31-3P 459831-32-4P (Continued) 459831-32-4P RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective preparation of N5-substituted sulfahydantoins via reductive

alkylation of resin-bound phenylalanine with substituted benzaldehydes and subsequent sulfamoylation, resin-cleavage, and cyclization)

RN 283587-14-4 RAPAIUS

CN 1.2.5-Thiadiazolidin-3-one,

5-[(4-methoxyphenyl)methyl)-4-(phenylmethyl)-,

1,1-dioxide, (45)- (9C) (CA INDEX NAME)

Absolute stereochemistry.

459831-30-2 KCAPLUS
Benzonitrile, 4-[([35)-1,1-dioxido-4-oxo-3-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

459831-31-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-nitrophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-32-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphenyl)methyl)-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 Oct 2001
ACCESSION NUMBER: 2001:735235 HCAPLUS
DOCUMENT NUMBER: 136:85785
TITLE: A one-step protocol for the N-chloromethylation of heterocyclic imides
AUTHOR(S): He, Shu; Yu, Hongyi; Fu, Qinghong; Kuang, Rongze;

AUTHOR(S): Epp,

CORPORATE SOURCE:

Department of Chemistry, Wichita State University, Wichita, Ms, 67260, USA

SOURCE:

SOURCE:

SOURCE:

PUBLISHER:

Harcel Dekker, Inc.

DOCUMENT TYPE:

LANGUAGE:

CASREACT 136:85785

A A convenient single step methodol. for the N-chloromethylation of heterocyclic imides using a mixture of formaldehyde sodium bisulfite adduct

and thionyl chloride is described. For example, the chloromethylation of 5-Butyl-3-propyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide gave. 387859-83-8 387859-86-1 RACT (Reactant or reagent) (preparation of 2-(chloromethyl-1,2,5-thiadiazolidin-3-one by chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 387859-83-8 HCAPLUS 1,2,5-thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 387859-86-1 HCAPLUS CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9P 387859-88-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

387859-88-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 5-(chloromethyl)-4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

$$\begin{array}{c|c} \text{CH}_2-\text{Ph} \\ \\ \text{Ph}-\text{CH}_2 \\ \\ \text{N} \\ \\ \text{O} \\ \\ \text{CH}_2-\text{N}-\text{C}-\text{OMe} \\ \\ \text{O} \\ \\ \\ \text{S}-\text{Ph} \\ \end{array}$$

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl)(methylsulfonyl)-, butyl ester (9C1) (CA INDEX

220869-14-7 HCAPLUS Carbamic acid,

220869-16-9 HCAPLUS

[2-[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 13 Jun 2001 ACCESSION NUMBER: 2001:426029 HCAPLUS DOCUMENT NUMBER: 115:2826655

TITLE: Inhibition of serine protesses by functionalized sulfonamides coupled to the

1.2.5-thiadiazolidin-3-one

ne
1,1 dioxide scaffold
Groutas, W. C.; He, S.; Kuang, R.; Ruan, S.; Tu, J.;
Chan, H.-K.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic 4 Medicinal Chemistry (2001), 9(6),
1543-1548 AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER :

DOCUMENT TYPE:

1543-1548
CODEN: BMECEP; ISSN: 0968-0896
ISHER: Elsevier Science Ltd.
MENT TYPE: Journal
UAGE: English
A challenge associated with drug design is the development of selective inhibitors of proteases (serine or cysteine) that exhibit the same

(Uses)
(inhibition of serine proteases by functionalized sulfonamides coupled to 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)
220889-05-6 HCAPLUS
Carbamic acid, [{1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-y1|methyl1|(methylsulfonyl)amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 365216-39-3 HCAPLUS
CN Benzamide,
N-[[4-(2-methylpropyl]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

365216-41-7 HCAPLUS

Glycine,
[[[(4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carbonyl]-, ethyl-ester
(9CI) (CA INDEX NAME)

365216-42-8 HCAPLUS

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Carbamic acid, {[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl}(phenylsulfonyl)-, butyl ester (9CI) (CA
INDEX
NAME)

RN 365216-43-9 HCAPLUS CN L-Phenylalanine, N-[[[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-

(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carb onyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

35

REFERENCE COUNT: THIS THERE ARE 35 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 283587-15-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-16-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-18-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[4{rrifluoromethyl}phenyl]methyl]-, 1,1-dioxide, (45)- (9CI)

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued I.2.5-Thiadiazolidin-3-one, 5-{(2,3-dihydro-1,4-benzodioxin-6-yl)methyl}-4-{(-methylethyl)-,1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (dS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-22-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 283587-24-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(2-(methylthio)ethyl]-, 1,1-dioxide, (4S]- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-35-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((3-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-36-7 HCAPLUS
CN Acetamide, N-[4-[[(3S)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-37-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(6-nitro-1,3-benzodioxol-5-yl)methyl)-,1,1-dioxide,(45)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-42-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[[4[phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI)- (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-43-6 HCAPLUS
CN Acetamide, N-{4-[(135)-1,1-dioxido-4-oxo-3-[[4-(phenylmethoxy)phenyl]methyl)-1,2,5-thiadiazolidin-2-yl]methyl}phenyl]-(9CI) (CA IMDEX NAME)

Absolute stereochemistry.

RN 346697-44-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(6-nitro-1,3-benzodioxol-5-y1]methyl]-4-[[4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 346697-38-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-39-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl]phenyl]methyl]4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-40-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl}-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-41-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[[4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 346697-45-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl)-4-[[4-(phenylmethoxyl)henyl]methyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-46-9 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one,
5-[(2,4-dimethoxy)-methylphenyl]methyl]-4-[[4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

RN 346697-47-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[2-[methylthio]ethyl]-, 1,1-dioxide, (45)- [9CI] (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

346697-48-1 RCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

RN 346697-49-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl]-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

RN 346697-50-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl]phenyl]methyl]4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
346697-55-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(6-nitro-1,3-benzodioxol-5-yl]methyl]-4[([phenylmethyl)thio]methyl), 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-56-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-57-2 HCAPLUS
1,2,5-Thiadiarollidine-3-acetic acid, 2-[(3-chlorophenyl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-58-3 HCAPLUS
1,2,5-Thiadizolidine-3-acetic acid, 2-[[4-(acetylamino)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (38)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-51-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one,'5-[(2-chlorophenyl)methyl]-4[(jbertylmethyl)thio]methyl]-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

346697-53-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

346697-54-9 HCAPLUS
Acetamide, N-{4-[{(3R)-1,1-dioxido-4-oxo-3-[{(phenylmethyl)thio]methyl}-1,2,5-thiadiazolidin-2-yl]methyl}phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid,
2-[(4-chloro-3-nitrophenyl)methyl]-4oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-60-7 HCAPLUS
1,2,5-Thiadiazolidine-3-scetic acid, 2-[(2,4-dimethoxy-3-methylphenyl)methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

RN ' 346697-62-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

$$\underbrace{ \begin{array}{c} H \\ N \\ \end{array} }_{S} \underbrace{ \begin{array}{c} O \\ O \\ \end{array} }_{C1}$$

RN 346697-63-0 HCAPLUS
(N 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-64-1 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 4-(1-methylethyl)-5-[(3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-65-2 HCAPLUS
CN Benzoic acid, 4-[[(3S)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-73-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-chloro-5-(trifluoromethyl]phenyl]methyl]-4-[[4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 346697-74-3 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[[1-(phenylmethyl]-1H-imidazol-4-yl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-[[1-(phenylmethyl)-1H-imidazol-4-yl]methyl]- L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-69-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[(4(phenylmethoxylphenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-71-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[[4-(phenylmethoxy)phenyl]methyl]-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-72-1 HCAPLUS
CN 1,2,5-Thiadiezolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-y1)methyl]-4[(4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-76-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[[1-(phenylmethyl)-1H-imidazol-4-yl]methyl]-, 1,1-dioxide, (45)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 346697-77-6 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-methylphenyl)methyl]-4-oxo-,
methyl ester, 1,1-dioxide, (33)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-79-8 HCAPLUS

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-[[4(trifluoromethyl)phenyl]methyl)-, methyl ester, 1,1-dioxide, (3S)- [9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 346697-80-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-{(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4-oxo-, methyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-81-2 HCAPLUS
CN Acetamide, N-[4-[[(3S)-3-[2-(methylthio)ethyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-82-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[2-(methylthio)ethyl]-5-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-, 1,1-dioxide, (4s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(4-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-88-9 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CI INDEX

Absolute stereochemistry.

4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-03-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chlorophenyl)methyl]-4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-84-5 HCRPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl]-4[((phenylmethyl)thio)methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-85-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl]phenyl]methyl]4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-89-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (38)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 346697-91-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-{(phenylmethoxy)methyl}-5-{{3-{rrifluoromethyl}phenyl}methyl}-, 1,1-dioxide, (45)- (SCI) (CA INDEX NAMP)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-92-5 HCAPLUS
Benzoic acid, 4-{{(3S)-1,1-dioxido-4-oxo-3-{(phenylmethoxy)methyl}-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester (9CI) (CA INDEX NAM2)

346697-93-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{{2,3-dichlorophenyl}methyl}-4{{phenylmethoxy}methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

346697-97-0 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346698-03-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-phenyl-5-[(2-(trifluoromethyl)phenyl)methyl)-, 1,1-dioxide, (43)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346698-04-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-[[3-[trifluoromethyl]phenyl]methyl], 1,1-dioxide, (45)- (9CI) CA INDEX NAME)

Absolute stereochemistry.

346698-05-3 HCAPLUS
Benzoic acid, 4-[(35)-1,1-dioxido-4-oxo-3-phenyl-1,2,5-thiadiazolidin-2yllmethyll-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-99-2 HCAPLUS
Benzoic acid, 4-[(3S)-3-[(4-nitrophenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

346698-00-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-[(4-nitrophenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346698-06-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-phenyl-1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

346698-12-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{4-methoxyphenyl}methyl]-4-{{1S}-1-methylpropyl}-, 1,1-dioxide, {45}- (9CI) (CA INDEX NAME)

346698-14-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4-[(1S)-1-methylpropyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: THIS

THERE ARE 47 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 22 Dec 2000 ACCESSION NUMBER: 2000:998004 HCAPLUS DOCUMENT NUMBER: 134:307088 1 2 5 5 7 7 7

134:307088
1,2,5-Thiadiazolidin-3-one 1,1 Dioxide: A Powerful Scaffold for Probing the S' Subsites of (Chymo)trypsin-Like Serine Proteases Groutas, William C.; Epp, Jeffrey B.; Kuang, Rongze; Ruan, Sumei; Chong, Lee S.; Venkataraman, Radhika;

Tu,

Juan; He, Shu; Yu, Hongyi; Fu, Qinghong; Li, Yue He;
Truong, Tien M.; Vu, Nga T.

CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA

SOURCE: Archives of Biochemistry and Biophysics (2001),
385(1), 162-169
CODEN: ABBIA4; ISSN: 0003-9861

PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: Agglish
B The 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) embodies a motif
that allows it to dock to the active site of (chymo)trypsin-like

in a predictable and substrate-like fashion. Consequently, inhibitors derived from this heterocyclic scaffold interact with both the S and S subsites of an enzyme. Exploitation of binding interactions with both

S and S' subsites of a target enzyme may lead to compds, with greatly enhanced enzyme selectivity and inhibitory potency. This preliminary report describes the use of a series of compds, having the heterocyclic scaffold linked to various amino acids to probe the S' subsites of human leukocyte elastase (HLE), proteinase 3 (PR 3), and cathepsin G (Cat G). For comparative purposes, a series of compds, derived from a related scaffold, isothiazolidin-3-one 1,1 dioxide (II), was also generated. Several of the compds, were found to be highly potent and selective time-dependent inhibitors of HLE, PR 3, and Cat G. (c) 2001 Academic

Press.
334975-68-7P 334975-69-8P 334975-75-6P 334975-85-8P 334975-88-1P

RL: BAC (Biological activity or effector, except adverse); BSU

logical study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (BiOLogical study); PREP (Preparation) (1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold for probing S' subsites of human leukocyte elastase, proteinase 3 and cathepsin G) 334975-68-7 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

-со2н

334975-81-4 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, ((4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-83-6 HCAPLUS L-Phenylalanine, ((4S)-1,1-dioxido-3-oxo-4.5-bis(phenylmethyl)-1,2,5 thiadiazolidin-2-yl]methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HC1

1.4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

334975-69-8 HCAPLUS
D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-75-6 HCAPLUS
L-Phenylalanine, [(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 334975-74-5 CMF C23 H29 N3 O5 S

Absolute stereochemistry

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

334975-88-1 HCAPUS
D-Phenylalanine, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: THERE ARE 24 CITED REFERENCES AVAILABLE FOR

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220869-27-2 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl-2-oxazoly1)thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-[{(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 19 Jul 2000 ACCESSION NUMBER: 2000:488727 HCAPLUS

DOCUMENT NUMBER:

2000:30072. Inchange 133:277919 Potent inhibition of serine protesses by heterocyclic sulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1 TITLE:

AUTHOR(S):

AUTHOR(S):

BH, S.; Kuang, R.; Venkataraman, R.; Tu, J.; Truong,
T. M.; Chan, H. K.; Groutas, M. C.

Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA

Bioorganic 4 Medicinal Chemistry (2000), B(7),
1713-1717

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER:
PUBLISHER:
PUBLISHER:
BLisevier Science Ltd.
Journal
LANGUAGE:
English
OTHER SOURCE(S):
CASREACT 133:277919

AB The existence of subtle differences in the Sn' subsites of closely-related
(chymo)trypsin-like serine proteases, and the fact that the
1,2,5-thiadjarolidin-3-one 1,1 dioxide scaffold docks to the active site of (chymo)trypsin-like enzymes in a substrate-like feshion, suggested that

that the introduction of recognition elements that can potentially interact with the Sn' subsites of these proteases might provide an effective means for optimizing enzyme potency and selectivity. Accordingly, a series of heterocyclic sulfide derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (1) was synthesized and the inhibitory activity and selectivity of these compost. toward human leukocyte elastase (HLE), proteinase 3 (PR 3) and cathepsin G (Cat G) were then determined Compds. with Pl=isobutyl were found to be potent, time-dependent inhibitors of HLE and.

Pl-isobutyl were found to be potent, time-dependent inhibitors of HLE and, to a lesser extent PR 3, while those with Pl-benzyl inactivated Cat G rapidly and irreversibly. This study has demonstrated that 1,2,5-thiadiazolidin-3-one 1,1 dioxide-based heterocyclic sulfides are effective inhibitors of (chymoltrypsin-like serine proteases.

IT 220869-26-1P 220869-32-0P 220869-33-9-8P 220869-30-7P 220869-33-9-52P 220869-33-9-5P 220869-33-9-5P 220869-30-9P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study); PREP (Preparation) potent inhibition of serine proteases by heterocyclic sulfide derivs. of thiadiazolidinone dioxide)

RN 220869-26-1 RCRPLUS

CN 12,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 220869-30-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2-Ph

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-2-([(5-phenyl-2-benzoxazolyl)thio]methyl]-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-39-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4,5-bis(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-40-9 HCAPIUS .

1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-benzoxazolyl)thio|methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

IT

300553-85-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of thiadiazolidinone dioxide derivative; potent inhibition

serine proteases by heterocyclic sulfide derivs. of thiadiazolidinone dioxide)

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 15 Jun 2000 ACCESSION NUMBER: 2000:395930 HCAPLUS DOCUMENT NUMBER: 133:159638

TITLE:

Utilization of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold in the design of potent inhibitors

AUTHOR (S):

serine proteases: SAR studies using carboxylates Kuang, R., Epp, J. B.; Ruan, S.; Chong, L. S.; Venkataraman, R.; Tu, J.; He, S.; Truong, T. M.; Gettes, W. Department of Chemistry, Wichita State University, Wichita, KS 67260, USA Bioorganic & Medicinal Chemistry (2000), 8(5), 1005-1016 CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd. PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

MENT TYPE: Journal
UAGE: English
A series of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one
1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds has been
synthesized and the inhibitory profile of these compds. toward human
leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3) was
then determined Most of the compds. were found to be potent,

then determined Most of the compds. were found to be potent, -dependent inhibitors of elastase, with some of the compds. exhibiting kinact/KI values as high as 4,928,300 M-l s-1. The inhibitory potency of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform was found to be influenced by both the pKa and the inherent structure of the leaving group. Proper selection of the primary specificity group was found to lead to selective inhibition of HLE over Cat G, however, those compds. that inhibited HLE also inhibited PR 3, albeit less efficiently. The predictable mode of binding of these ds.

ds.

suggests that, among closely-related serine proteases, highly selective inhibitors of a particular serine protease can be fashioned by exploiting subtle differences in their S' subsites.

247179-63-1P 287921-30-6P 287921-33-9P 287921-73-79 287921-73-79 287921-73-8P 287921-73-8P 287921-82-92 287921-

RL: BAC (Biological activity or effector, except adverse); BSU

logical study, unclassified); SPN (Synthetic preparation); BIOL (Biological study), PREP (Preparation) (synthesis of thiadiazolidinone dioxides and isothiazolidinone

as serine protease inhibitors)
247179-63-1 HCAPLUS

4411/3-63-1 HCARPUN 1,2,5-Thisdiazolidin-3-one, 2-[(acetyloxy)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-30-6 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[4-ethyl-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-33-9 HCAPLUS
Benzeneacetic acid, 4-{[(35)-5-[(2,2-dimethyl-1-oxopropoxy)methyl]-1,1-dioxido-4-oxo-3-propyl-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 287921-37-3 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

, L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

287921-38-4 HCAPLUS
Benzeneacetic acid, 4-[[(3S)-5-[{2,2-dimethyl-1-oxopropoxy)methyl]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI)(CA INDEX NAME)

Absolute stereochemistry.

AGINGLIBUTE REALITY (45) - (ACCEYLORY) METHY] -4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-42-0 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 2-{(benzoyloxy)methyl]-4-{2-methylpropyl}-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzenepropanoic acid, [(4S)-4-(2-methylpropyl)-1,l-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-54-4 HCAPLUS
Benzeneacetic acid, [(45)-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-65-7 HCAPLUS
Benzoic acid, 2,6-dichloro-,
-,1-dioxido-3-oxo-4,5-bis[phenylmethyl]1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-91-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{acetyloxy}methy1]-4,5-bis(phenylmethy1)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-45-3 HCAPLUS

Senzoic acid, 2,6-dichloro-,
[(48)-4-(2-methylpropy)-1,1-dioxido-3-oxo-5[phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-46-4 HCAPLUS
Benzeneacetic acid, 4-[[(3S)-5-[[(2,6-dichlorobenzoyl)oxy]methyl]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-52-2 HCAPLUS

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

212331-98-1P 212331-99-2P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxides and isothiazolidinone ΙT

dioxides

ides
as serine protease inhibitors)
212331-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylthio)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 44 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 May 2000
ACCESSION NUMBER: 2000:324184 HCAPLUS
DOCUMENT NUMBER: 133:105000
TITLE: Solid-phase synthesis of sulfahydantoins
Albericio, Fernando; Garcia, Javier; Michelotti,
Enrique L.: Nicolas, Ernesto: Tice, Colin M.
Department of Organic Chemistry, University of
Barcelons, Barcelons, 08028, Spain
Tetrahedron Letters (2000), 41(17), 3161-3163
CODEN: TELEATY ISSN: 0040-4039
PUBLISHER: Disevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 133:105000
OTHER SOURCE(S): CASREACT 133:105000
AB A 5-step solid-phase synthesis of 2-unsubstituted 1, 2, 5-thiadiarolidin-3one 1, I-dioxides, sulfahydantoins, from Nu-Facc amino acids and
aromatic aldehydes is described. The key step is the base-mediated
cyclitive

aromatic aldehydes is described. The key step is the Dass-med cyclitive cleavage of a resin bound Nu-maintosulfonyl Nu-benzyl amino acid to afford the desired product. This synthesis allows the diverse library of compds. based on this heterocycle.

IT 203567-14-4P 203587-15-59 203587-16-6P 203567-18-6P 203587-19-9 203567-22-4P 203587-24-6P 203567-22-4P 203567-22-4P 203567-24-6P 203567-34-6P 2

Absolute stereochemistry.

1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,1,1-dioxide (9CI) (CA INDEX NAME)

203587-24-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-((2-chlorophenyl)methyl)-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1.4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

283587-16-6 HCAPLUS 1, 2, 5-Thiadiazolidin-3-one, 1-methyletchyl)-5-[(3-methylphenyi)methyl]-, 1, 1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-{{4-(trifluoromethyl)phenyl}methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN . 283587-19-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dihydro-1,4-benzodioxin-6-y1)methy1}-4-{1-methylethy1}-, 1,1-dioxide, {45}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 27 Aug 1999
ACCESSION NUMBER: 1999:536684 HCAPLUS
DOCUMENT NUMBER: 131:296963
ITITLE: 131:296963
AUTHOR(S): Human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold Groutes, William C.; Schechter, Norman M., He, Shu; Yu, Hongyi; Huang, Peng; Tu, Juan
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1999), 9(15), 2199-2204
CODEN: BMCLEB: 15SN: 0960-894X
EUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANCUAGE: English
AB A series of compds. that utilize the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold was synthesized and shown to be highly effective inhibitors of recombinant human skin chymase..
IT 170918-99-7 247178-61-2 247179-63-1
247179-64-2 247179-64-6 247179-66-4
247179-70-0 247179-71-75-5 247179-76-6
RL: BBAC (Biological activity or effector, except adverse); BSU
(Biological Study, unclassified); PRP (Properties); BIOL (Biological study) (human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)
RN 170918-99-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
CN Acetic acid, hydroxy-,
[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

RN 247179-66-4 HCAPLUS CN Propanoic acid, 2-hydroxy-, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-67-5 HCAPLUS
Benzenescetic acid, o-hydroxy-, [(4S)-1,1-dioxido-3-oxo-4,5-bis (phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl ester (9CI) (CA INDEX

Absolute stereochemistry.

1.4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{{acetyloxy}methyl}-4,5-bis{phenylmethyl}-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-64-2 HCAPLUS
Propanedioic acid, mono[[{4S}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl}-1,2,5-thiadiazolidin-2-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-65-3 HCAPLUS

ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

247179-60-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(methylsulfonyl)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

247179-69-7 HCAPLUS
Acetic acid, [[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

247179-70-0 HCAPLUS Propanoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN Absolute stereochemistry. (Continued)

247179-71-1 HCAPLUS
Benzoic acid, 2-{{{(4S}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl}sulfonyl}- (9CI) (CA INDEX NAME)

247179-72-2 HCAPLUS
Benzoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yllmethyl)aulfonyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

(Continued) ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-74-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-75-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-benzoxazoly1)thio]methy1]-4,5-bis(phenylmethy1)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-76-6 HCAPIUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-{{(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 25 Aug 1999
ACCESSION NUMBER: 1999:529836 HCAPLUS
DOCUMENT NUMBER: 131:296959
TITLE: A General Inhibitor Scaffold for Serine Proteases
with

DOCUMENT NOMBER:

A General Inhibitor Scaffold for Serine Proteases

a (Chymo)trypsin-Like Fold: Solution-Phase
Construction and Evaluation of the First Series of Libraries of Mechanism-Based Inhibitors

AUTHOR(S):

Kuang, Rongre: Epp. Jeffrey B.; Ruan, Sumei; Yu,
Hongyir Huang, Beng; He, Shu; Tu, Juan; Schechter,
Norman M.: Turbov, Jane: Froelich, Christopher J.;
Groutas, William C.

CORPORATE SOURCE:

Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Journal of the American Chemical Society (1999),
121(35), 8128-8129
CODEN: JACSAT; ISSN: 0002-7863

American Chemical Society

DOCUMENT TYPE:
Journal
LANGUAGE:
AB The authors demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1 dioxide
platform embodies a general motif that renders the platform capable of
binding to the active site of many serine proceases with a
(chymo)trypsin-like fold in a predictable fashion and is amenable to the
facile construction of libraries for lead identification and
optimization.

1 170918-99-7P 170919-03-6P 189124-02-5P
247178-39-8P 247178-40-1P 247178-41-2P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPM (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)
(inhibitor; general inhibitor scaffold for serine proteases with a
construction and
of first series of libraries of mechanism-based inhibitors)

evaluation

of first series of libraries of mechanism-based inhibitors)

RN 170918-99-7 HCAPLUS

CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, {45}- (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN Absolute stereochemistry. (Continued)

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylmethyl)-2-([phenylsulfonyl)methyl]-4propyl-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-39-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{4-aminobutyl}-5-(phenylmethyl)-2[(phenylwlfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 16 Mar 1999 ACCESSION NUMBER: 1999:172588 HCAPLUS DOCUMENT NUMBER: 130:209985 TITLE: Preserve

130:209985
Preparation of 1,2,5-thiadiarolidin-3-one 1,1-dioxide derivatives as serine protease inhibitors Groutas, William C., Kuang, Rongze Wichita State University, USA PCT Int. Appl., 69 pp.
CODEN: PIXXD2
Patent English 1
1

WO 1998-U517406

W 19980821

INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 9909977 A1 19990304 WO 1998-US17406 19980821
W: AU, BR, CA, IS, JP, MX, NZ
RW: AT, BE, CH. CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE

US 6420401 B1 20020716 US 1997-916693 19970822
AU 9890298 A 19990316 AU 1998-90298 19980821
EP 1011668 A1 20000628 EP 1998-942192 19980821
R: DE, GB
PRIORITY APPLN. INFO.: US 1997-916693 A 19970822

OTHER SOURCE(S):

MARPAT 130:209985

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247178-40-1 HCAPLUS

1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-5-[(phenylsulfonyl)methyl)-, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[[(45}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- G, H; m = 1-2; each R7 = amino acid side chain; each R8, R9 = alkyl, aryl, aralkyl, alkaryl, heterocyclyl; each R10-R15 = H, any group R8;

R16, R17 = heterocyclylalkyl; R18 = any group R8, NHR19; R19 = alkyl, aryl, aralkyl; with provisos], oligomers and combinatorial libraries contg. them, and methods of using them, are disclosed. Thus, title

contg. them, and methods of using them, are disclosed. Thus, title d.

If showed apparent second-order rate consts. Kinact/KI (M-1s-1) of 119,360, 27,400, and 60 for inhibition of human leukocyte elastase, proteinase 3, and cathepsin G, resp., by in vitro assays. 220868-74-6DP, combinatorial library derivs. 220868-93-DP, combinatorial library derivs. 220868-81 library derivs. 220868-81-1DP, combinatorial library derivs. 220868-81-1DP, combinatorial library derivs. 220868-87-DP, combinatorial library derivs. 220868-97-DP, combinatorial library derivs. 220868-98-7-DP, combinatorial library derivs. 220868-97-DP, combinatorial library derivs. 220868-98-PP, combinatorial library derivs. 220869-98-9P, combinatorial library derivs. 220869-98-56P 220869-98-PP 220869-07-8P 220869-19-P 220869-19-PP 220869-19-PP 220869-19-PP 220869-20-PP 220869-19-PP 220869-20-PP 220869-33-OP 220869-27-PP 220869-33-OP 220869-33-OP 220869-33-OP 220869-33-OP 220869-33-OP 220869-38-PP 220869-38-P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (Use) (preparation of amino acid-derived thiadiazolidinone dioxide derivs.

as serine protease inhibitors)
RN 220868-74-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(4-methoxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ÇH2C1

RN 220868-75-7 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 2-(chloromethyl)-5-((3-phenoxyphenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2C1

RN 220868-80-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2-OAC

RN 220868-81-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(3phenoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

O = S-Me

CH2-N-C-OME

O N

CH2

CH2

Pho

Absolute stereochemistry.

RN 220868-92-8 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

MeO N S H S CO2H C1

RN 220868-93-9 HCAPLUS
CN L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl][9CI]
(GCA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2 OAC

RN 220868-86-0 HCAPLUS
Carbamic acid, [[5-{(4-methoxyphenyl)methyl}-1,1-dioxido-3-oxo-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

O= 5-Me

CH2-N-C-OMe

CH2-N-C-OMe

CH2-N-C-OMe

RN 220868-87-1 HCAPLUS
Cn Carbamic acid, [[1,1-dioxido-3-oxo-5-[{3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) [CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220868-98-4 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl}sulfonyl}methyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220868-99-5 HCAPLUS

N L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[[3-phenoxyphenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl)methyl](9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester [9CI) (CA INDEX NAME)

220869-06-7 HCAPLUS
Carbanic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, phenylmethyl ester (9CI)
(CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220869-16-9 HCAPLUS
CN Carbamic acid,
[2-{[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-chiadiacolidin-2-yl]methyl)|methylsulfonyl)amino]-2-oxoethyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

RN 220869-19-2 HCAPLUS
CN Glycine,
[[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl][phenylsulfonyl)amino[carbonyl]-, ethyl ester
(9C1) (CA INDEX NAME)

220869-20-5 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2,2'-methylenebis(4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester (9CI) (CA

INDEX NAME)

RN 220869-14-7 HCAPLUS
CN Carbamic acid,
[2-{[[4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiarolidin-2-yl|methyl](methylsulfonyl)amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-26-1 HCAPLUS
1,2,5-Thiadizolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4-(2-methylpropyl)-5-[phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 220869-27-2 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl2-2-oxazoly1)thio]methyl]-4-[2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1.2.5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-[{(5-

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contphenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) NAME)

220869-30-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-40-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-benzoxazoly1)thio]methy1]-4,5-bis[phenylmethy1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220859-41-0 HCAPLUS 1,2,5-Thiadiarolidine-2-acetic acid, α -fluoro-3-oxo-4,5-bis[phenylmethyl]-, ethyl ester, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-64-7 220869-65-8 RL: RCT (Reactant)/ RRCT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derive. IT

serine protesse inhibitors) 220869-64-7 HCAPLUS

1.2.5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-2-[{(5-phenyl-2-benzoxzolyl)thio|methyl}-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-39-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-65-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

220869-61-4P 220869-62-5P 220869-63-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide deriva. IT

serine protease inhibitors)
220859-61-4 HCAPLUS
1.2.5-Thiadiarolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dimethylethyl ester, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

220869-62-5 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-63-6 HCAPLUS 1,2,5-Thiadiazolidine-2-acetamide, 4-(2-methylpropyl)-3-oxo-N-(2-phenylethyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 212331-98-1 KCAPLUS 1,2,5-Thiodatarolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-(phenylthio)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212332-00-8 HCAPLUS
Benzeneacetic acid, 3-[((35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX

Absolute stereochemistry

IT 212331~79-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3) 212331-79-8 HCAPLUS

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 05 Aug 1998 ACCESSION NUMBER: 1998:487562 HCAPLUS DOCUMENT NUMBER: 129:216561

DOCUMENT NUMBER: TITLE:

129:216561
Potent and specific inhibition of human leukocyte elastase, cathepsin G and proteinase 3 by sulfone derivatives employing the 1,2.5-thiadiazolidin-3-one 1,1-dioxide scaffold Groutas, William C.; Kuang, Rongze; Ruan, Sumei; Epp, Jeffrey B.; Venkataraman, Radhika; Truong, Tien M. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Bioorganic 6 Medicinal Chemistry (1998), 6(6), AUTHOR (S): CORPORATE SOURCE:

SOURCE: 661-671

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd. PUBLISHER:

DOCUMENT TYPE: LANGUAGE: Journal English

This paper describes the results of structure-activity relationship studies in a series of heterocyclic mechanism-based inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold (1; R1 = iso-6benzyl; R2 = Bu, Me, benzyl; R2 = Bu, Me, benzyl; R2 = Bozeh, SOZC6H4Cl-4, etc.) and capable of interacting with the Sn and S'n subsites of a serine proteinase. Sulfone derivs. of I were found to be highly effective, time-dependent inhibitors of human leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3). The judicious selection of an R1 group (accommodated at the primary specificity site S1) that is based on the known substrate specificity of a target serine proteinase, was found to yield highly selective inhibitors. The presence of a benzyl group (R2 = benzyl) at the S2 subsite was found to lead to a pronounced enhancement

inhibitory potency. Furthermore, the effective use of computer graphics and modeling has led to the design of potent, water-soluble inhibitors.

The results of these studies demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1-dioxide platform provides an effective means for appending recognition elements in a well-defined vector relationship, and in fashioning highly-selective and potent inhibitors of serime proteinases.

IT 212331-98-1P 212331-99-2P 212332-00-8P

RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) [1,2,5-thiadiazolidin-3-one 1,1-dioxide inhibitors of human leukocyte elastase, cathepsin G and proteinase 3)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on SIN (Continued)
Benzoic acid, 3-[[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

IT 170918-99-7P 170919-01-4P 170919-03-6P
212331-77-6P 212331-78-7P 212331-80-1P
212331-81-2P 212331-82-3P 212331-83-4P
212331-86-7P 212331-89-8P 212331-95-8P
212331-92-5P 212331-94-7P 212331-95-8P
212331-97-0P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3)
RN 170918-99-7 MCAPUUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2((phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

170919-01-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one,
(phenylmethyl)-5-([25]-3-phenyl-2-propenyl)2-[(phenylmulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Ph S Ph

RN 170919-03-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 212331-77-6 HCAPLUS

Senzoic acid, 4-[[(35)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
[9C1] (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-78-7 HCAPLUS
CN Benzoic acid, 4-[[(35)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-82-3 HCAPLUS
CN Benzoic acid, 2-[{(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-83-4 HCAPLUS
CN Benzeneacetic acid, 4-[(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[[(4-chlorophenyl)sulfonyl]methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 212331-80-1 HCAPLUS

Benzoic acid, 3-[[(35)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-81-2 HCAPLUS
CN Benzoic acid, 2-[[(38)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued Absolute stereochemistry.

RN 212331-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(2-phenylethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[{4-chlorophenyl)methyl]sulfonyl]methyl]-4(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

212331-92-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-2-{{{3-phenylpropyl}sulfonyl}methyl}-, 1,1-dioxide, (4S)- {9CI} (CA INDEX NAME)

212331-94-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-{{[3-(trifluoromethyl)phenyl]sulfonyl]methyl}-, 1,1-dioxide, (45)- (9CI) · (CA INDEX NAME) RN CN

Absolute stereochemistry.

212331-95-8 HCAPLUS 212331-95-E MCAPAGE 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 09 Apr 1998 ACCESSION NUMBER: 1998:200895 HCAPLUS DOCUMENT NUMBER: 128:278642

TITLE:

128:278642
Use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent inhibitors of serine proteinases Kuang, Rongze: Venkataraman, Radhika: Ruan, Sumei: Groutas, William C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1998), AUTHOR(S):

CORPORATE SOURCE:

SOURCE: 8(5),

539-544 CODEN: BMCLE8; ISSN: 0960-894X Elsevier Science Ltd. Journal

PUBLISHER:

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The attachment of a phosphate leaving group to the
1,2,5-thiadiazolidin-3one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds was found
to yield highly potent, time-dependent inhibitors of human leukocyte
elastase (HLE).
205932-85-0P 205932-87-2P 205932-88-3P
205932-89-4P
205932

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (use of the 1.2,5-thiediacolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent

inhibitors of serine proteinases) 205932-85-0 HCAPLUS

205932-85-0 HCAPLUS
Phosphoric acid, dimethyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX

205932-87-2 HCAPLUS
Phosphoric acid, dibutyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

212331-97-0 HCAPLUS
Benzeneacetic acid, 4-{[(3S}-1,1-dioxido-4-oxo-3-(phenylmethyl)-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

205932-88-3 HCAPLUS
Phosphoric acid, [4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl bis(phenylmethyl), ester (9CI) (CA INDEX NAME)

205932-89-4 HCAPLUS
Phosphoric acid, [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl diphenyl ester (9CI) (CA INDEX NAME)

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 30 Aug 1997
ACCESSION NUMBER: 1997:555602 HCAPLUS
DOCUMENT NUMBER: 127:257045

TITLE: Competitive particle concentration fluorescence immunoassays for measuring antidiabetic drug levels

mouse plasma
Bright, Stuart, W.; Tinsley, Frank C.; Dominianni,
Samuel J.; Schmiegel, Klaus K.; Fitch, Lora L.; Gold,
Gerald
Lilly Research Laboratories, Eli Lilly and Company,
Indianapolis, IN, 46285, USA
Journal of Immunological Methods (1997), 207(1), AUTHOR (S)

CORPORATE SOURCE:

CODEN: JIMMBG; ISSN: 0022-1759

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

CRY TYPE: Journal NACE: English Two competitive particle concentration fluorescence immunoassays were developed

loped to measure blood levels of analogs of antidiabetic drugs being tested in diabetic mice. Ligands that contained the active pharmacophores were conjugated to PPD for immunization and to β -phycoerythrin for use as a tracer in the immunoassays. Approx. 90% of 262 compds. assayed were detectable at less than 120 nM in plasma which was well below the

iated therapeutic level of 1 µM for lowering blood glucose. These data were used to define the bioavailability of test compds. and assist in decisions

sions
of constructing active analogs. Of addnl. interest, we noted
crossreactivity of one monoclonal antibody for 3 different compound

ses
that are all known to bind with varying affinities to peroxisome
proliferator-activated receptors.
196079-43-3
RE: ANT (Analyte): ANST (Analytical study)
(competitive particle concentration fluorescence immunoassays for

measuring
antidiabetic drug levels in mouse plasma)
RN 156079-43-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[2-(2-phenyl-4-oxažolyl)ethoxy]phenyl)-,
1,1-dioxide (SCI) (CA INDEX NAME)

- Bilanzo

FORMAT

THERE ARE 13 CITED REFERENCES AVAILABLE FOR 13

REFERENCE COUNT: THIS

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN
ED Entered STN: 09 Apr 1997
ACCESSION NUMBER: 1997:226843 HCAPLUS
DOCUMENT NUMBER: 126:287561
TITLE: Structure-Based Design of a Gene

Structure-Based Design of a General Class of Mechanism-Based Inhibitors of the Serine Proteinases

Mechanism-Based Inhibitors of the Serine Proteinases
Employing a Novel Amino Acid-Derived Heterocyclic
Scaffold
AUTHOR(S): Groutas, William C.; Kuang, Rongre; Venkataraman,
Radhika; Epp, Jeffrey B.; Ruan, Sumei; Prakash, Om
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
SOURCE: Biochemistry (1997), 36(16), 4739-4750
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We describe in this paper the structure-based design of a general class
of

PUBLISHER: DOCUMENT TYPE:

heterocyclic mechanism-based inhibitors of the serine proteinases that embody in their structure a novel peptidomimetic scaffold (1,2,5-thiadiazolidin-3-one 1,1-dioxide). Sulfone derivs. of this class were time-dependent, potent, and highly efficient irreversible inhibitors of human leukocyte elestase, cathepsin G, and proteinase 3. The partition

ratios for a select number of inhibitors were found to range between 0 and 1.

We furthermore demonstrate that these inhibitors exhibit remarkable

We furthermore demonstrate that these inhibitors exhibit remarkable enzyme
selectivity that is dictated by the nature of the Pl residue and is
consistent with the known substrate specificity reported for these
enzymes. Thus, inhibitors with small hydrophobic side chains were
effective inhibitors of elastase, those with aromatic side chains of
cathepsin G, and those with a basic side chain of bovine trypsin. Taken
together, the findings cited herein reveal the emergence of a general
class of stable mechanism-based inhibitors of the serine proteinases
which

or can be readily synthesized using amino acid precursors. Biochem. and high-field NNR studies show that the interaction of this class of inhibitors with a serine proteinase results in the formation of a stable acyl complex(es) and the release of benzenesulfinate, formaldehyde, and a low mol. weight heterocycle. The data are consistent with initial

formation
of a Michaelis-Menten complex, acylation of Ser195, and tandem loss of

leaving group. The initial HLE-inhibitor complex reacts with water generating formaldehyde and a stable HLE-inhibitor complex. Whether the initial HLE-inhibitor complex also reacts with His57 to form a third complex is not known at this point. The desirable salient parameters associated with this class of inhibitors, including the expeditious generation of structurally diverse libraries of inhibitors based on I, suggest that this class of mechanism-based inhibitors is of general applicability and can be used in the development of inhibitors of human and viral serime proteinases of clin. relevance. 170918-99-79 170919-90-36F 189124-00-79 189124-00-79 [89124-02-89 [89124-04-79 [89124-06-99]]

BAC (Biological activity or effector, except adverse); BSU

R1: BAC (Biological activity or effector, except adverser, but (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and structure activity relations of mechanism-based inhibitors

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) of human leukocyte serine proteinases employing a novel amino acid-derived heterocyclic scaffold)
170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylmulfonyl)methyl]-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

189124-00-3 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 4-ethyl-5-(phenylmethyl)-2-((phenylmulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

189124-02-5 HCAPLUS

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN CN 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-2-([phenylmulfonyl)methyl]-4-propyl-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

189124-04-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-06-9 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 4-butyl-5-(phenylmethyl)-2-((phenylmulfonyl)methyl)-, 1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 01 Dec 1995 ACCESSION NUMBER: 1995:954574 HCAPLUS DOCUMENT NUMBER: 123:340140 123:340140
Novel serine protease inhibitors: derivatives of isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide Groutas, William C. Wichita State University, USA PCT Int. Appl., 93 pp. CODEN: PIXXD2
Patent TITLE: INVENTOR(S) PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: English 1 FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.					KIN	D	DATE		APPLICATION NO.						DATE			
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									3 WO 1995-US236										
		W:	AM,	AT,	AU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	ES,	FI,	GB,	
			GE,	HU,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LK,	LT,	LU,	LV,	MD,	MG,	MN,	MW,	
			NL.	NO.	NZ.	PL.	PT,	RO.	RU,	SD,	SE,	SI,	SK,	TJ,	TT,	UA,	υz,	VN	
		RW:	AT.	BE.	CH.	DE.	DK.	ES.	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE	
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		6863																	
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	EP 739338																		
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SE			,																
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	AŤ	2159	38			T		2002	0415			995-							
	NZ	3297	66			А		2001	0223		NZ 1	998-	3297	66		1	9980	216	
PRIO		APP									US 1	994-	1773	52		A 1	9940	103	
										,	WO 1	995-	US 2 3	6	,	W 1	9950	103	

MARPAT 123:340140 OTHER SOURCE(S):

Various isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide derivs., e.g. I [X=CR2, (un)] substituted NH; Rl = H, alkyl, (un) substituted NH; Rl = H, alkyl, (un) substituted benzyl, indolylalkyl, etc.; Y=non-steroidal antiinfilammatory residue, H, protected amino acid, acyloxy, etc.], and their use to reduce or inhibit the activity of serime proteases, are claimed. The compost are useful as anti-infilammatory and anti-metastatic agents. For example, 4-benzylisothiazolidin-3-one 1,1-dioxide underwent

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
N-alkylation with CLCH2SPh and Et3N in MeCN, followed by S-oxidn. with
m-ClC6H4C(0)00H in CH2Cl2 (90%), to give title compd. II. In an in vitro
assay, II had an apparent 2nd-order inactivation rate const. (kobs/[I]

M-1
s-333, If and an apparent 2nd-other tracted control of the state o

Absolute stereochemistry. Double bond geometry as shown.

IT 170919-15-OP
R1: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-15-O HCAPUUS
CN 1,2,5-Thiadiazolidin-3-one,
4,5-bis(phenylacthyl)-2-[(phenylthio)methyl]-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 153044-45-2P 170918-99-7P 170919-01-4P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) study, unclassified), SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
153044-45-2 HCAPLUS
1,2,5-Thadiazolidino-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170918-99-7 HCAPLUS
1,2,5-Thisdiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(phenylaethyl)-5-[(2E)-3-phenyl-2-propenyl]2-{(phenylsulfonyl)methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

170919-22-9 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 170919-03-6 170919-21-8 170919-22-9
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study);

USES (Uses)

(Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-03-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-21-8 HCAPLUS .
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-(phenylsulfonyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:124451 HCAPLUS
DOCUMENT NUMBER: 120:124451
TITLE: Substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides:
a new class of potential mechanism-based inhibitors

of

AUTHOR (S)

CORPORATE SOURCE:

human leukocyte elastase and cathepsin G Groutas, William C.; Kuang, Rongze; Venkataraman, Radhika Dep. Chem., Wichita State Univ., Wichita, KS, 67260, USA Biochemical and Biophysical Research Communications (1994), 198(1), 341-9 CODEN: BBRCA9; ISSN: 0006-291X Journal English

DOCUMENT TYPE: LANGUAGE: GI

A series of substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides (I, R = benzyl; Rl = H, Me, benzyl, CH2Co2-tert-Bu or CH2Co2-benzyl) was prepd, and their in vitro inhibitory activity toward human leukocyte elastase

and

cathepsin G was investigated. These compds. inactivated the 2 enzymes efficiently and in a time-dependent fashion.

IT 153044-45-29
RL: SPN [Synthetic preparation]; PREP (Preparation)
(preparation of and human leukocyte elastase and cathepsin G inhibition by)
RN 153044-45-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis{phenylmethyl}-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 26 Jan 1991
ACCESSION NUMBER: 1991:23940 HCAPLUS
DOCUMENT NUMBER: 114:23940
INTRA and intermolecular α-sulfamidoalkylation reactions

AUTHOR(S): Lee, Chai Ho; Kohn, Harold
CORPORATE SOURCE: Dep. Chem., Univ. Houston, TX, 77204-5641, USA

USA Journal of Organic Chemistry (1990), 55(25), 6098-104 CODEN: JOCEAH; ISSN: 0022-3263 Journal English CASREACT 114:23940 SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(5): GI

The utility of $\alpha\text{-sulfamidoalkylation}$ processes for the generation of sulfamides has been examined. Both intra- and intermol. $\alpha\text{-}$ sulfamidoalkylation transformations were observed to proceed in moderate

good yields. The generality of these processes has been demonstrated using N.N'-dl(aryl-substituted) sulfamides, and the utility of these reactions was examined for the preparation of cyclic sulfamides of novel structure. Thus, reaction of PhCH2NISCO3NE2 with ECOZCCH(OE)2 in the presence of CF3CO2H gave 74% dithiatetrarocinedicarboxylate tetraoxide I, whereas reaction of 3-MeOC6H4CH2NH5O2NH2 with ECOZCCH(OE)2 in CF3CO2H followed by methylation gave benzothiadiazepinecarboxylate dioxide II. The crystal structures of I and II were determined 130670-00-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of) 130670-00-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-hydroxy-5-(2-phenylethyl)-, 1,1-dioxide, menosodium salt (SCI) (CA INDEX NAME)

ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

• Na

130669-99-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of)
130669-99-7 HCAPLUS
1,2,5-Thiadiazolidine-3,4-dione, 2-(2-phenylethyl)-, 1,1-dioxide, sodium salt (9CI) (CA INDEX NAME)

• Na

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION		
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